

Hexanedioic acid, bis(2-methylpropyl) ester

Other names:	Adipic acid bis(2-methylpropyl) ester Adipic acid, diisobutyl ester Bis(2-methylpropyl) hexanedioate DIBA Diisobutyl hexanedioate Ftaflex DIBA Hexanedioic acid, 1,6-bis(2-methylpropyl) ester Hexanedioic acid, diisobutyl ester Isobutyl adipate NSC 6343 Plasthall DIBA adipic acid diisobutyl ester diisobutyl adipate diisobutyl adipate [DIBA] hexanedioic acid bis(2-methylpropyl) ester
Inchi:	InChI=1S/C14H26O4/c1-11(2)9-17-13(15)7-5-6-8-14(16)18-10-12(3)4/h11-12H,5-10H2,1
InchiKey:	RDOFJDLLWVCMRU-UHFFFAOYSA-N
Formula:	C14H26O4
SMILES:	CC(C)COC(=O)CCCC(=O)OCC(C)C
Mol. weight [g/mol]:	258.35
CAS:	141-04-8

Physical Properties

Property code	Value	Unit	Source
gf	-405.72	kJ/mol	Joback Method
hf	-832.45	kJ/mol	Joback Method
hfus	30.54	kJ/mol	Joback Method
hvap	64.29	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.945		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	1652.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1680.00		NIST Webbook

rinpol	1699.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1691.00		NIST Webbook
ripol	2132.00		NIST Webbook
ripol	2119.00		NIST Webbook
tb	671.42	K	Joback Method
tc	852.27	K	Joback Method
tf	361.86	K	Joback Method
vc	0.856	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.34	J/molxK	852.27	Joback Method
cpg	696.05	J/molxK	822.13	Joback Method
cpg	683.00	J/molxK	791.99	Joback Method
cpg	669.19	J/molxK	761.84	Joback Method
cpg	654.60	J/molxK	731.70	Joback Method
cpg	639.24	J/molxK	701.56	Joback Method
cpg	623.10	J/molxK	671.42	Joback Method
dvisc	0.0018500	Paxs	348.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0029200	Paxs	323.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)

dvisc	0.0026400	Paxs	328.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0024000	Paxs	333.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0021900	Paxs	338.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0020100	Paxs	343.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0032400	Paxs	318.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)

dvisc	0.0017100	Paxs	353.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0015900	Paxs	358.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0014800	Paxs	363.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0013800	Paxs	368.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0012900	Paxs	373.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)

dvisc	0.0036300	Paxs	313.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0040900	Paxs	308.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0046500	Paxs	303.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0053300	Paxs	298.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0061700	Paxs	293.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)

dvisc	0.0072200	Paxs	288.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0085600	Paxs	283.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C141048&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Phase behavior of diisobutyl adipate carbon dioxide mixtures:	https://www.doi.org/10.1016/j.fluid.2006.07.013
Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates):	https://www.doi.org/10.1021/je100237h
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure

rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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