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)CCCCC(=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	1657.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1691.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1656.00		NIST Webbook

rinpol	1655.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1680.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1660.00		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	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	623.10	J/mol×K	671.42	Joback Method
cpg	639.24	J/mol×K	701.56	Joback Method
cpg	654.60	J/mol×K	731.70	Joback Method
cpg	669.19	J/mol×K	761.84	Joback Method
cpg	683.00	J/mol×K	791.99	Joback Method
cpg	696.05	J/mol×K	822.13	Joback Method
cpg	708.34	J/mol×K	852.27	Joback Method
dvisc	0.0036300	Pa×s	313.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0072200	Pa×s	288.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)

dvisc	0.0061700	Pa×s	293.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)	
dvisc	0.0053300	Pa×s	298.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)	
dvisc	0.0046500	Pa×s	303.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)	
dvisc	0.0040900	Pa×s	308.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)	
dvisc	0.0085600	Pa×s	283.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)	

dvisc	0.0032400	Pa×s	318.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0029200	Pa×s	323.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0026400	Pa×s	328.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0024000	Pa×s	333.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0021900	Pa×s	338.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)

dvisc	0.0020100	Pa×s	343.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)	
dvisc	0.0018500	Pa×s	348.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)	
dvisc	0.0017100	Pa×s	353.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)	
dvisc	0.0015900	Pa×s	358.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)	
dvisc	0.0014800	Pa×s	363.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)	

dvisc	0.0013800	Pa×s	368.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)
dvisc	0.0012900	Pa×s	373.15	Influence of the Molecular Structure on the Volumetric Properties and Viscosities of Dialkyl Adipates (Dimethyl, Diethyl, and Diisobutyl Adipates)

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C141048&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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