

Adipic acid, isobutyl 2-methylpent-3-yl ester

Inchi:	InChI=1S/C16H30O4/c1-6-14(13(4)5)20-16(18)10-8-7-9-15(17)19-11-12(2)3/h12-14H,6-
InchiKey:	RQPWSDGFMWEQKU-UHFFFAOYSA-N
Formula:	C16H30O4
SMILES:	CCC(OC(=O)CCCC(=O)OCC(C)C)C(C)C
Mol. weight [g/mol]:	286.41

Physical Properties

Property code	Value	Unit	Source
gf	-391.32	kJ/mol	Joback Method
hf	-879.01	kJ/mol	Joback Method
hfus	32.20	kJ/mol	Joback Method
hvap	68.36	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.724		Crippen Method
mcvol	251.180	ml/mol	McGowan Method
pc	1436.98	kPa	Joback Method
rinpol	1804.00		NIST Webbook
rinpol	1804.00		NIST Webbook
tb	716.74	K	Joback Method
tc	899.00	K	Joback Method
tf	369.40	K	Joback Method
vc	0.962	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.04	J/molxK	716.74	Joback Method
cpg	752.23	J/molxK	747.12	Joback Method
cpg	768.53	J/molxK	777.49	Joback Method
cpg	783.94	J/molxK	807.87	Joback Method
cpg	798.48	J/molxK	838.25	Joback Method
cpg	812.14	J/molxK	868.62	Joback Method
cpg	824.95	J/molxK	899.00	Joback Method
dvisc	0.0024183	Paxs	369.40	Joback Method

dvisc	0.0009093	Paxs	427.29	Joback Method
dvisc	0.0004318	Paxs	485.18	Joback Method
dvisc	0.0002403	Paxs	543.07	Joback Method
dvisc	0.0001497	Paxs	600.96	Joback Method
dvisc	0.0001014	Paxs	658.85	Joback Method
dvisc	0.0000731	Paxs	716.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353557&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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