

Diglycolic acid, isobutyl 2-octyl ester

Inchi:	InChI=1S/C16H30O5/c1-5-6-7-8-9-14(4)21-16(18)12-19-11-15(17)20-10-13(2)3/h13-14H
InchiKey:	AZDLUJNDJGTHKC-UHFFFAOYSA-N
Formula:	C16H30O5
SMILES:	CCCCCCC(C)OC(=O)COCC(=O)OCC(C)C
Mol. weight [g/mol]:	302.41

Physical Properties

Property code	Value	Unit	Source
gf	-493.88	kJ/mol	Joback Method
hf	-1005.95	kJ/mol	Joback Method
hfus	36.91	kJ/mol	Joback Method
hvap	71.16	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.104		Crippen Method
mvol	257.050	ml/mol	McGowan Method
pc	1410.13	kPa	Joback Method
rmpol	2342.00		NIST Webbook
rmpol	2342.00		NIST Webbook
tb	739.60	K	Joback Method
tc	920.56	K	Joback Method
tf	406.63	K	Joback Method
vc	0.986	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.62	J/molxK	739.60	Joback Method
cpg	781.34	J/molxK	769.76	Joback Method
cpg	797.17	J/molxK	799.92	Joback Method
cpg	812.09	J/molxK	830.08	Joback Method
cpg	826.12	J/molxK	860.24	Joback Method
cpg	839.25	J/molxK	890.40	Joback Method
cpg	851.49	J/molxK	920.56	Joback Method
dvisc	0.0012606	Paxs	406.63	Joback Method

dvisc	0.0005594	Paxs	462.12	Joback Method
dvisc	0.0002955	Paxs	517.62	Joback Method
dvisc	0.0001766	Paxs	573.12	Joback Method
dvisc	0.0001156	Paxs	628.61	Joback Method
dvisc	0.0000810	Paxs	684.11	Joback Method
dvisc	0.0000599	Paxs	739.60	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382317&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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