

Diglycolic acid, isobutyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C16H30O5/c1-12(2)8-20-14(17)10-19-11-15(18)21-9-13(3)7-16(4,5)6/h12-13H
InchiKey:	IXSSWDGPHCXOGO-UHFFFAOYSA-N
Formula:	C16H30O5
SMILES:	CC(C)COC(=O)COCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	302.41

Physical Properties

Property code	Value	Unit	Source
gf	-491.04	kJ/mol	Joback Method
hf	-1014.70	kJ/mol	Joback Method
hfus	29.50	kJ/mol	Joback Method
hvap	69.86	kJ/mol	Joback Method
log10ws	-2.61		Crippen Method
logp	2.818		Crippen Method
mcvol	257.050	ml/mol	McGowan Method
pc	1430.46	kPa	Joback Method
rinpola	2262.00		NIST Webbook
rinpola	2262.00		NIST Webbook
tb	736.37	K	Joback Method
tc	922.89	K	Joback Method
tf	409.05	K	Joback Method
vc	0.975	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	766.52	J/molxK	736.37	Joback Method
cpg	841.95	J/molxK	891.80	Joback Method
cpg	828.75	J/molxK	860.71	Joback Method
cpg	814.61	J/molxK	829.63	Joback Method
cpg	799.54	J/molxK	798.54	Joback Method
cpg	783.51	J/molxK	767.46	Joback Method
cpg	854.24	J/molxK	922.89	Joback Method
dvisc	0.0000495	Paxs	736.37	Joback Method

dvisc	0.0000685	Paxs	681.82	Joback Method
dvisc	0.0001004	Paxs	627.26	Joback Method
dvisc	0.0001581	Paxs	572.71	Joback Method
dvisc	0.0002740	Paxs	518.16	Joback Method
dvisc	0.0005406	Paxs	463.60	Joback Method
dvisc	0.0012784	Paxs	409.05	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=U382037&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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