

Diglycolic acid, 3,7-dimethyloctyl isobutyl ester

Inchi:	InChI=1S/C18H34O5/c1-14(2)7-6-8-16(5)9-10-22-17(19)12-21-13-18(20)23-11-15(3)4/h1
InchiKey:	ZSLBLPWDUXONMC-UHFFFAOYSA-N
Formula:	C18H34O5
SMILES:	CC(C)CCCC(C)CCOC(=O)COCC(=O)OCC(C)C
Mol. weight [g/mol]:	330.46

Physical Properties

Property code	Value	Unit	Source
gf	-479.48	kJ/mol	Joback Method
hf	-1052.51	kJ/mol	Joback Method
hfus	38.57	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.598		Crippen Method
mvol	285.230	ml/mol	McGowan Method
pc	1233.74	kPa	Joback Method
rmpol	2577.00		NIST Webbook
rmpol	2577.00		NIST Webbook
tb	784.92	K	Joback Method
tc	969.58	K	Joback Method
tf	414.17	K	Joback Method
vc	1.091	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.95	J/molxK	784.92	Joback Method
cpg	899.52	J/molxK	815.70	Joback Method
cpg	916.05	J/molxK	846.47	Joback Method
cpg	931.55	J/molxK	877.25	Joback Method
cpg	946.01	J/molxK	908.03	Joback Method
cpg	959.45	J/molxK	938.80	Joback Method
cpg	971.86	J/molxK	969.58	Joback Method
dvisc	0.0012351	Paxs	414.17	Joback Method

dvisc	0.0004857	Paxs	475.96	Joback Method
dvisc	0.0002367	Paxs	537.75	Joback Method
dvisc	0.0001338	Paxs	599.55	Joback Method
dvisc	0.0000841	Paxs	661.34	Joback Method
dvisc	0.0000573	Paxs	723.13	Joback Method
dvisc	0.0000414	Paxs	784.92	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=U382144&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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