Diglycolic acid, isobutyl nonyl ester

Inchi: InChI=1S/C17H32O5/c1-4-5-6-7-8-9-10-11-21-16(18)13-20-14-17(19)22-12-15(2)3/h15H
InchiKey: MNOMARDZEZXEBH-UHFFFAOYSA-N
Formula: C17H32O5
SMILES: CCCCCCCCCOC(=O)COCC(=O)OCC(C)C
Mol. weight [g/mol]: 316.43

Physical Properties

Property code	Value	Unit	Source
gf	-483.02	kJ/mol	Joback Method
hf	-1021.31	kJ/mol	Joback Method
hfus	43.02	kJ/mol	Joback Method
hvap	73.77	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.496		Crippen Method
mcvol	271.140	ml/mol	McGowan Method
pc	1306.12	kPa	Joback Method
rinpol	2579.00		NIST Webbook
rinpol	2579.00		NIST Webbook
tb	762.92	K	Joback Method
tc	943.28	K	Joback Method
tf	432.90	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.07	J/mol×K	762.92	Joback Method
cpg	839.00	J/mol×K	792.98	Joback Method
cpg	855.01	J/mol×K	823.04	Joback Method
cpg	870.08	J/mol×K	853.10	Joback Method
cpg	884.23	J/mol×K	883.16	Joback Method
cpg	897.46	J/mol×K	913.22	Joback Method
cpg	909.76	J/mol×K	943.28	Joback Method
dvisc	0.0009338	Pa×s	432.90	Joback Method

dvisc	0.0004495	Pa×s	487.90	Joback Method
dvisc	0.0002509	Pa×s	542.91	Joback Method
dvisc	0.0001559	Pa×s	597.91	Joback Method
dvisc	0.0001050	Pa×s	652.91	Joback Method
dvisc	0.0000752	Pa×s	707.92	Joback Method
dvisc	0.0000565	Pa×s	762.92	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=U382132&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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