

Diglycolic acid, 3-methylbutyl octyl ester

Inchi:	InChI=1S/C17H32O5/c1-4-5-6-7-8-9-11-21-16(18)13-20-14-17(19)22-12-10-15(2)3/h15H
InchiKey:	IVTDOLABIWCOBZ-UHFFFAOYSA-N
Formula:	C17H32O5
SMILES:	CCCCCCCCOC(=O)COCC(=O)OCCC(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
mvol	271.140	ml/mol	McGowan Method
pc	1306.12	kPa	Joback Method
rinpol	2589.00		NIST Webbook
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tb	762.92	K	Joback Method
tc	943.28	K	Joback Method
tf	432.90	K	Joback Method
vc	1.048	m ³ /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	Paxs	432.90	Joback Method

dvisc	0.0004495	Paxs	487.90	Joback Method
dvisc	0.0002509	Paxs	542.91	Joback Method
dvisc	0.0001559	Paxs	597.91	Joback Method
dvisc	0.0001050	Paxs	652.91	Joback Method
dvisc	0.0000752	Paxs	707.92	Joback Method
dvisc	0.0000565	Paxs	762.92	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382274&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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