

Diglycolic acid, heptyl 3-methylbutyl ester

Inchi:	InChI=1S/C16H30O5/c1-4-5-6-7-8-10-20-15(17)12-19-13-16(18)21-11-9-14(2)3/h14H,4-
InchiKey:	JCSPPTKSKSSMGH-UHFFFAOYSA-N
Formula:	C16H30O5
SMILES:	CCCCCCCOC(=O)COCC(=O)OCCC(C)C
Mol. weight [g/mol]:	302.41

Physical Properties

Property code	Value	Unit	Source
gf	-491.44	kJ/mol	Joback Method
hf	-1000.67	kJ/mol	Joback Method
hfus	40.44	kJ/mol	Joback Method
hvap	71.54	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	3.106		Crippen Method
mvol	257.050	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2467.00		NIST Webbook
rinpol	2467.00		NIST Webbook
tb	740.04	K	Joback Method
tc	919.24	K	Joback Method
tf	421.63	K	Joback Method
vc	0.992	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.13	J/molxK	740.04	Joback Method
cpg	780.67	J/molxK	769.91	Joback Method
cpg	796.34	J/molxK	799.77	Joback Method
cpg	811.14	J/molxK	829.64	Joback Method
cpg	825.07	J/molxK	859.51	Joback Method
cpg	838.12	J/molxK	889.37	Joback Method
cpg	850.30	J/molxK	919.24	Joback Method
dvisc	0.0010358	Paxs	421.63	Joback Method

dvisc	0.0005045	Paxs	474.70	Joback Method
dvisc	0.0002839	Paxs	527.77	Joback Method
dvisc	0.0001775	Paxs	580.84	Joback Method
dvisc	0.0001200	Paxs	633.90	Joback Method
dvisc	0.0000862	Paxs	686.97	Joback Method
dvisc	0.0000650	Paxs	740.04	Joback Method

Sources

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=U382273&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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