

Diglycolic acid, 3-methylbutyl propyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C12H22O5/c1-4-6-16-11(13)8-15-9-12(14)17-7-5-10(2)3/h10H,4-9H2,1-3H3

UVWZDSAEZCKQJG-UHFFFAOYSA-N

C12H22O5

CCCOC(=O)COCC(=O)OCCC(C)C

246.30

Physical Properties

Property code	Value	Unit	Source
gf	-525.12	kJ/mol	Joback Method
hf	-918.11	kJ/mol	Joback Method
hfus	30.07	kJ/mol	Joback Method
hvap	62.64	kJ/mol	Joback Method
log10ws	-1.42		Crippen Method
logp	1.545		Crippen Method
mcvol	200.690	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook
tb	648.52	K	Joback Method
tc	828.30	K	Joback Method
tf	376.55	K	Joback Method
vc	0.767	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.76	J/molxK	648.52	Joback Method
cpg	558.41	J/molxK	678.48	Joback Method
cpg	572.40	J/molxK	708.45	Joback Method
cpg	585.72	J/molxK	738.41	Joback Method
cpg	598.37	J/molxK	768.38	Joback Method
cpg	610.34	J/molxK	798.34	Joback Method
cpg	621.62	J/molxK	828.30	Joback Method
dvisc	0.0014862	Paxs	376.55	Joback Method

dvisc	0.0007629	Paxs	421.88	Joback Method
dvisc	0.0004458	Paxs	467.21	Joback Method
dvisc	0.0002864	Paxs	512.53	Joback Method
dvisc	0.0001977	Paxs	557.86	Joback Method
dvisc	0.0001443	Paxs	603.19	Joback Method
dvisc	0.0001101	Paxs	648.52	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U382267&Units=SI

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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