

Diglycolic acid, ethyl 3-methylbutyl ester

Inchi:	InChI=1S/C11H20O5/c1-4-15-10(12)7-14-8-11(13)16-6-5-9(2)3/h9H,4-8H2,1-3H3
InchiKey:	DAPTWARVVWXOPX-UHFFFAOYSA-N
Formula:	C11H20O5
SMILES:	CCOC(=O)COCC(=O)OCCC(C)C
Mol. weight [g/mol]:	232.27

Physical Properties

Property code	Value	Unit	Source
gf	-533.54	kJ/mol	Joback Method
hf	-897.47	kJ/mol	Joback Method
hfus	27.48	kJ/mol	Joback Method
hvap	60.41	kJ/mol	Joback Method
log10ws	-1.00		Crippen Method
logp	1.155		Crippen Method
mcvol	186.600	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpola	1860.00		NIST Webbook
rinpola	1860.00		NIST Webbook
tb	625.64	K	Joback Method
tc	806.61	K	Joback Method
tf	365.28	K	Joback Method
vc	0.712	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	491.99	J/molxK	625.64	Joback Method
cpg	556.04	J/molxK	776.45	Joback Method
cpg	544.48	J/molxK	746.29	Joback Method
cpg	532.28	J/molxK	716.13	Joback Method
cpg	519.46	J/molxK	685.96	Joback Method
cpg	506.03	J/molxK	655.80	Joback Method
cpg	566.96	J/molxK	806.61	Joback Method
dvisc	0.0001243	Paxs	625.64	Joback Method

dvisc	0.0001624	Paxs	582.25	Joback Method
dvisc	0.0002215	Paxs	538.85	Joback Method
dvisc	0.0003189	Paxs	495.46	Joback Method
dvisc	0.0004924	Paxs	452.07	Joback Method
dvisc	0.0008339	Paxs	408.67	Joback Method
dvisc	0.0016004	Paxs	365.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382266&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

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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