

Diglycolic acid, ethyl hexyl ester

Inchi:	InChI=1S/C12H22O5/c1-3-5-6-7-8-17-12(14)10-15-9-11(13)16-4-2/h3-10H2,1-2H3
InchiKey:	OVXSVUCTPMCRSL-UHFFFAOYSA-N
Formula:	C12H22O5
SMILES:	CCCCCOC(=O)COCC(=O)OCC
Mol. weight [g/mol]:	246.30

Physical Properties

Property code	Value	Unit	Source
gf	-522.68	kJ/mol	Joback Method
hf	-912.83	kJ/mol	Joback Method
hfus	33.60	kJ/mol	Joback Method
hvap	63.03	kJ/mol	Joback Method
log10ws	-1.66		Crippen Method
logp	1.690		Crippen Method
mcvol	200.690	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpola	2034.00		NIST Webbook
tb	648.96	K	Joback Method
tc	826.09	K	Joback Method
tf	391.55	K	Joback Method
vc	0.773	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.30	J/molxK	648.96	Joback Method
cpg	608.90	J/molxK	796.57	Joback Method
cpg	597.08	J/molxK	767.04	Joback Method
cpg	584.60	J/molxK	737.52	Joback Method
cpg	571.47	J/molxK	708.00	Joback Method
cpg	557.70	J/molxK	678.48	Joback Method
cpg	620.07	J/molxK	826.09	Joback Method
dvisc	0.0001185	Paxs	648.96	Joback Method
dvisc	0.0001522	Paxs	606.06	Joback Method

dvisc	0.0002032	Paxs	563.16	Joback Method
dvisc	0.0002846	Paxs	520.25	Joback Method
dvisc	0.0004234	Paxs	477.35	Joback Method
dvisc	0.0006812	Paxs	434.45	Joback Method
dvisc	0.0012164	Paxs	391.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382054&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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