

Diglycolic acid, hexyl pentyl ester

Inchi:	InChI=1S/C15H28O5/c1-3-5-7-9-11-20-15(17)13-18-12-14(16)19-10-8-6-4-2/h3-13H2,1-2
InchiKey:	SEFBOYDDFVHNEU-UHFFFAOYSA-N
Formula:	C15H28O5
SMILES:	CCCCCOC(=O)COCC(=O)OCCCCC
Mol. weight [g/mol]:	288.38

Physical Properties

Property code	Value	Unit	Source
gf	-497.42	kJ/mol	Joback Method
hf	-974.75	kJ/mol	Joback Method
hfus	41.37	kJ/mol	Joback Method
hvap	69.71	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.860		Crippen Method
mvol	242.960	ml/mol	McGowan Method
pc	1498.83	kPa	Joback Method
rinpol	2393.00		NIST Webbook
rinpol	2393.00		NIST Webbook
tb	717.60	K	Joback Method
tc	894.31	K	Joback Method
tf	425.36	K	Joback Method
vc	0.942	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	706.75	J/molxK	717.60	Joback Method
cpg	722.68	J/molxK	747.05	Joback Method
cpg	737.83	J/molxK	776.50	Joback Method
cpg	752.18	J/molxK	805.96	Joback Method
cpg	765.73	J/molxK	835.41	Joback Method
cpg	778.49	J/molxK	864.86	Joback Method
cpg	790.45	J/molxK	894.31	Joback Method
dvisc	0.0009550	Paxs	425.36	Joback Method

dvisc	0.0005119	Paxs	474.07	Joback Method
dvisc	0.0003082	Paxs	522.77	Joback Method
dvisc	0.0002024	Paxs	571.48	Joback Method
dvisc	0.0001419	Paxs	620.19	Joback Method
dvisc	0.0001048	Paxs	668.89	Joback Method
dvisc	0.0000807	Paxs	717.60	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=U382057&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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