

Diglycolic acid, heptyl 2,4,4-trimethylpentyl ester

Inchi:	InChI=1S/C19H36O5/c1-6-7-8-9-10-11-23-17(20)14-22-15-18(21)24-13-16(2)12-19(3,4)5
InchiKey:	XMBCPBWMTMYLROH-UHFFFAOYSA-N
Formula:	C19H36O5
SMILES:	CCCCCCCOC(=O)COCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	344.49

Physical Properties

Property code	Value	Unit	Source
gf	-463.34	kJ/mol	Joback Method
hf	-1071.34	kJ/mol	Joback Method
hfus	40.79	kJ/mol	Joback Method
hvap	76.93	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	4.132		Crippen Method
mvol	299.320	ml/mol	McGowan Method
pc	1156.93	kPa	Joback Method
rinpol	2686.00		NIST Webbook
rinpol	2686.00		NIST Webbook
tb	805.45	K	Joback Method
tc	992.66	K	Joback Method
tf	457.86	K	Joback Method
vc	1.149	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.83	J/molxK	805.45	Joback Method
cpg	959.54	J/molxK	836.65	Joback Method
cpg	976.17	J/molxK	867.85	Joback Method
cpg	991.75	J/molxK	899.06	Joback Method
cpg	1006.28	J/molxK	930.26	Joback Method
cpg	1019.79	J/molxK	961.46	Joback Method
cpg	1032.30	J/molxK	992.66	Joback Method
dvisc	0.0007172	Paxs	457.86	Joback Method

dvisc	0.0003242	Paxs	515.79	Joback Method
dvisc	0.0001720	Paxs	573.72	Joback Method
dvisc	0.0001026	Paxs	631.65	Joback Method
dvisc	0.0000667	Paxs	689.59	Joback Method
dvisc	0.0000464	Paxs	747.52	Joback Method
dvisc	0.0000339	Paxs	805.45	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382042&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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