

Diglycolic acid, 3,7-dimethyloctyl pentyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-468.62	kJ/mol	Joback Method
hf	-1067.87	kJ/mol	Joback Method
hfus	44.68	kJ/mol	Joback Method
hvap	77.83	kJ/mol	Joback Method
log10ws	-4.10		Crippen Method
logp	4.132		Crippen Method
mvol	299.320	ml/mol	McGowan Method
pc	1148.32	kPa	Joback Method
rmpol	2755.00		NIST Webbook
rmpol	2755.00		NIST Webbook
tb	808.24	K	Joback Method
tc	993.75	K	Joback Method
tf	440.44	K	Joback Method
vc	1.153	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.23	J/molxK	808.24	Joback Method
cpg	1019.37	J/molxK	962.83	Joback Method
cpg	1005.88	J/molxK	931.91	Joback Method
cpg	991.34	J/molxK	900.99	Joback Method
cpg	975.71	J/molxK	870.08	Joback Method
cpg	959.02	J/molxK	839.16	Joback Method
cpg	1031.79	J/molxK	993.75	Joback Method
dvisc	0.0000389	Paxs	808.24	Joback Method

dvisc	0.0000529	Paxs	746.94	Joback Method
dvisc	0.0000760	Paxs	685.64	Joback Method
dvisc	0.0001174	Paxs	624.34	Joback Method
dvisc	0.0001993	Paxs	563.04	Joback Method
dvisc	0.0003849	Paxs	501.74	Joback Method
dvisc	0.0008930	Paxs	440.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382146&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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