

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

Inchi:	InChI=1S/C22H42O5/c1-6-7-8-9-10-11-12-13-14-26-20(23)17-25-18-21(24)27-16-19(2)1
InchiKey:	MTSCJTLFZJXXMX-UHFFFAOYSA-N
Formula:	C22H42O5
SMILES:	CCCCCCCCCOC(=O)COCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	386.57

Physical Properties

Property code	Value	Unit	Source
gf	-438.08	kJ/mol	Joback Method
hf	-1133.26	kJ/mol	Joback Method
hfus	48.56	kJ/mol	Joback Method
hvap	83.60	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	5.302		Crippen Method
mcvol	341.590	ml/mol	McGowan Method
pc	959.69	kPa	Joback Method
rinpola	3061.00		NIST Webbook
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tb	874.09	K	Joback Method
tc	1070.50	K	Joback Method
tf	491.67	K	Joback Method
vc	1.317	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.91	J/molxK	874.09	Joback Method
cpg	1143.60	J/molxK	906.83	Joback Method
cpg	1161.00	J/molxK	939.56	Joback Method
cpg	1177.16	J/molxK	972.30	Joback Method
cpg	1192.09	J/molxK	1005.03	Joback Method
cpg	1205.83	J/molxK	1037.77	Joback Method
cpg	1218.40	J/molxK	1070.50	Joback Method
dvisc	0.0004840	Paxs	491.67	Joback Method

dvisc	0.0002129	Paxs	555.41	Joback Method
dvisc	0.0001109	Paxs	619.14	Joback Method
dvisc	0.0000652	Paxs	682.88	Joback Method
dvisc	0.0000420	Paxs	746.62	Joback Method
dvisc	0.0000290	Paxs	810.35	Joback Method
dvisc	0.0000211	Paxs	874.09	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=U382045&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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