

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

Inchi:	InChI=1S/C23H44O5/c1-6-7-8-9-10-11-12-13-14-15-27-21(24)18-26-19-22(25)28-17-20(
InchiKey:	LAUHYMTYMWLVHX-UHFFFAOYSA-N
Formula:	C23H44O5
SMILES:	CCCCCCCCCOC(=O)COCC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	400.59

Physical Properties

Property code	Value	Unit	Source
gf	-429.66	kJ/mol	Joback Method
hf	-1153.90	kJ/mol	Joback Method
hfus	51.15	kJ/mol	Joback Method
hvap	85.83	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	5.692		Crippen Method
mcvol	355.680	ml/mol	McGowan Method
pc	905.06	kPa	Joback Method
tb	896.97	K	Joback Method
tc	1098.15	K	Joback Method
tf	502.94	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1187.23	J/molxK	896.97	Joback Method
cpg	1206.29	J/molxK	930.50	Joback Method
cpg	1223.97	J/molxK	964.03	Joback Method
cpg	1240.33	J/molxK	997.56	Joback Method
cpg	1255.37	J/molxK	1031.09	Joback Method
cpg	1269.16	J/molxK	1064.62	Joback Method
cpg	1281.71	J/molxK	1098.15	Joback Method
dvisc	0.0004222	Paxs	502.94	Joback Method
dvisc	0.0001842	Paxs	568.61	Joback Method
dvisc	0.0000954	Paxs	634.28	Joback Method

dvisc	0.0000559	Paxs	699.95	Joback Method
dvisc	0.0000359	Paxs	765.63	Joback Method
dvisc	0.0000247	Paxs	831.30	Joback Method
dvisc	0.0000180	Paxs	896.97	Joback Method

Sources

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=U382046&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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