Diglycolic acid, neopentyl tridecyl ester

Inchi: InChI=1S/C22H42O5/c1-5-6-7-8-9-10-11-12-13-14-15-16-26-20(23)17-25-18-21(24)27-1
InchiKey: YJDIYDAJCTVGCW-UHFFFAOYSA-N
Formula: C22H42O5
SMILES: CCCCCCCCCCCCCOC(=O)COCC(=O)OCC(C)(C)C
Mol. weight [g/mol]: 386.57

Physical Properties

Property code	Value	Unit	Source
gf	-435.64	kJ/mol	Joback Method
hf	-1127.98	kJ/mol	Joback Method
hfus	52.08	kJ/mol	Joback Method
hvap	83.99	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.447		Crippen Method
mcvol	341.590	ml/mol	McGowan Method
pc	954.96	kPa	Joback Method
rinpol	3128.00		NIST Webbook
rinpol	3128.00		NIST Webbook
tb	874.53	K	Joback Method
tc	1070.79	K	Joback Method
tf	506.67	K	Joback Method
vc	1.323	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1124.45	J/mol×K	874.53	Joback Method
cpg	1205.50	J/mol×K	1038.08	Joback Method
cpg	1191.71	J/mol×K	1005.37	Joback Method
cpg	1176.74	J/mol×K	972.66	Joback Method
cpg	1160.56	J/mol×K	939.95	Joback Method
cpg	1143.14	J/mol×K	907.24	Joback Method
cpg	1218.13	J/mol×K	1070.79	Joback Method
dvisc	0.0000231	Pa×s	874.53	Joback Method

dvisc	0.0000312	Pa×s	813.22	Joback Method
dvisc	0.0000442	Pa×s	751.91	Joback Method
dvisc	0.0000667	Pa×s	690.60	Joback Method
dvisc	0.0001089	Pa×s	629.29	Joback Method
dvisc	0.0001979	Pa×s	567.98	Joback Method
dvisc	0.0004155	Pa×s	506.67	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U381925&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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