Diglycolic acid, hexadecyl neopentyl ester

Inchi: InChI=1S/C25H48O5/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-29-23(26)20-28-21-2
InchiKey: OYXIZPXUQXRCFV-UHFFFAOYSA-N
Formula: C25H48O5
SMILES: CCCCCCCCCCCCCCCCCOC(=O)COCC(=O)OCC(C)(C)C
Mol. weight [g/mol]: 428.65

Physical Properties

Property code	Value	Unit	Source
gf	-410.38	kJ/mol	Joback Method
hf	-1189.90	kJ/mol	Joback Method
hfus	59.85	kJ/mol	Joback Method
hvap	90.67	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	6.617		Crippen Method
mcvol	383.860	ml/mol	McGowan Method
pc	805.25	kPa	Joback Method
rinpol	3467.00		NIST Webbook
rinpol	3467.00		NIST Webbook
tb	943.17	K	Joback Method
tc	1157.86	K	Joback Method
tf	540.48	K	Joback Method
vc	1.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.06	J/mol×K	943.17	Joback Method
cpg	1397.72	J/mol×K	1122.08	Joback Method
cpg	1383.78	J/mol×K	1086.30	Joback Method
cpg	1368.39	J/mol×K	1050.52	Joback Method
cpg	1351.51	J/mol×K	1014.73	Joback Method
cpg	1333.08	J/mol×K	978.95	Joback Method
cpg	1410.26	J/mol×K	1157.86	Joback Method
dvisc	0.0000142	Pa×s	943.17	Joback Method

dvisc	0.0000193	Pa×s	876.06	Joback Method
dvisc	0.0000276	Pa×s	808.94	Joback Method
dvisc	0.0000420	Pa×s	741.83	Joback Method
dvisc	0.0000696	Pa×s	674.71	Joback Method
dvisc	0.0001290	Pa×s	607.60	Joback Method
dvisc	0.0002783	Pa×s	540.48	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U381927&Units=SI
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

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