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

Inchi: InChI=1S/C26H50O5/c1-6-7-8-9-10-11-12-13-14-15-16-17-18-30-24(27)21-29-22-25(28)

InchiKey: GMNADRHTZPXYAU-UHFFFAOYSA-N

Formula: C26H50O5

SMILES: CCCCCCCCCCCCCCOC(=O)COCC(=O)OCC(C)CC(C)(C)C

Mol. weight [g/mol]: 442.67

Physical Properties

Property code	Value	Unit	Source
gf	-404.40	kJ/mol	Joback Method
hf	-1215.82	kJ/mol	Joback Method
hfus	58.92	kJ/mol	Joback Method
hvap	92.51	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.863		Crippen Method
mcvol	397.950	ml/mol	McGowan Method
pc	766.49	kPa	Joback Method
rinpol	3520.00		NIST Webbook
rinpol	3520.00		NIST Webbook
tb	965.61	K	Joback Method
tc	1187.20	K	Joback Method
tf	536.75	K	Joback Method
vc	1.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1377.22	J/mol×K	965.61	Joback Method
cpg	1397.58	J/mol×K	1002.54	Joback Method
cpg	1416.22	J/mol×K	1039.47	Joback Method
cpg	1433.19	J/mol×K	1076.41	Joback Method
cpg	1448.55	J/mol×K	1113.34	Joback Method
cpg	1462.35	J/mol×K	1150.27	Joback Method
cpg	1474.65	J/mol×K	1187.20	Joback Method
dvisc	0.0002765	Pa×s	536.75	Joback Method

dvisc	0.0001178	Pa×s	608.23	Joback Method
dvisc	0.0000601	Pa×s	679.70	Joback Method
dvisc	0.0000348	Pa×s	751.18	Joback Method
dvisc	0.0000222	Pa×s	822.66	Joback Method
dvisc	0.0000152	Pa×s	894.13	Joback Method
dvisc	0.0000110	Pa×s	965.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382049&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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