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

Inchi: InChI=1S/C24H46O5/c1-6-7-8-9-10-11-12-13-14-15-16-28-22(25)19-27-20-23(26)29-18-

InchiKey: CLPQMVLJUCHCMN-UHFFFAOYSA-N

Formula: C24H46O5

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

Mol. weight [g/mol]: 414.62

Physical Properties

Property code	Value	Unit	Source
gf	-421.24	kJ/mol	Joback Method
hf	-1174.54	kJ/mol	Joback Method
hfus	53.74	kJ/mol	Joback Method
hvap	88.06	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	6.083		Crippen Method
mcvol	369.770	ml/mol	McGowan Method
pc	854.96	kPa	Joback Method
rinpol	3297.00		NIST Webbook
rinpol	3297.00		NIST Webbook
tb	919.85	K	Joback Method
tc	1126.76	K	Joback Method
tf	514.21	K	Joback Method
vc	1.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1250.09	J/mol×K	919.85	Joback Method
cpg	1269.55	J/mol×K	954.34	Joback Method
cpg	1287.53	J/mol×K	988.82	Joback Method
cpg	1304.09	J/mol×K	1023.31	Joback Method
cpg	1319.25	J/mol×K	1057.79	Joback Method
cpg	1333.06	J/mol×K	1092.28	Joback Method
cpg	1345.56	J/mol×K	1126.76	Joback Method
dvisc	0.0003674	Pa×s	514.21	Joback Method

dvisc	0.0001590	Pa×s	581.82	Joback Method
dvisc	0.0000819	Pa×s	649.42	Joback Method
dvisc	0.0000478	Pa×s	717.03	Joback Method
dvisc	0.0000306	Pa×s	784.64	Joback Method
dvisc	0.0000211	Pa×s	852.24	Joback Method
dvisc	0.0000153	Pa×s	919.85	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=U382047&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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