Diglycolic acid, di(3,7-dimethyloctyl) ester

Inchi: InChI=1S/C24H46O5/c1-19(2)9-7-11-21(5)13-15-28-23(25)17-27-18-24(26)29-16-14-22(
InchiKey: KGGWTGSVRQHMFF-UHFFFAOYSA-N
Formula: C24H46O5
SMILES: CC(C)CCCC(C)CCOC(=O)COCC(=O)OCCC(C)CCCC(C)C
Mol. weight [g/mol]: 414.62

Physical Properties

Property code	Value	Unit	Source
gf	-431.40	kJ/mol	Joback Method
hf	-1181.63	kJ/mol	Joback Method
hfus	50.59	kJ/mol	Joback Method
hvap	88.19	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	5.794		Crippen Method
mcvol	369.770	ml/mol	McGowan Method
pc	857.47	kPa	Joback Method
rinpol	3241.00		NIST Webbook
rinpol	3241.00		NIST Webbook
tb	921.76	K	Joback Method
tc	1129.10	K	Joback Method
tf	466.79	K	Joback Method
vc	1.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1251.34	J/mol×K	921.76	Joback Method
cpg	1270.83	J/mol×K	956.32	Joback Method
cpg	1288.74	J/mol×K	990.87	Joback Method
cpg	1305.07	J/mol×K	1025.43	Joback Method
cpg	1319.86	J/mol×K	1059.98	Joback Method
cpg	1333.12	J/mol×K	1094.54	Joback Method
cpg	1344.88	J/mol×K	1129.10	Joback Method
dvisc	0.0006643	Pa×s	466.79	Joback Method

dvisc	0.0002274	Pa×s	542.62	Joback Method
dvisc	0.0001013	Pa×s	618.45	Joback Method
dvisc	0.0000538	Pa×s	694.28	Joback Method
dvisc	0.0000324	Pa×s	770.10	Joback Method
dvisc	0.0000214	Pa×s	845.93	Joback Method
dvisc	0.0000151	Pa×s	921.76	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=U382154&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