Diglycolic acid, 2,5-dimethylphenyl dodecyl ester

Inchi: InChI=1S/C24H38O5/c1-4-5-6-7-8-9-10-11-12-13-16-28-23(25)18-27-19-24(26)29-22-17

InchiKey: NMVXLHSROHKYDE-UHFFFAOYSA-N

Formula: C24H38O5

SMILES: CCCCCCCCCCCCOC(=O)COCC(=O)Oc1cc(C)ccc1C

Mol. weight [g/mol]: 406.56

Physical Properties

Property code	Value	Unit	Source
gf	-328.49	kJ/mol	Joback Method
hf	-946.92	kJ/mol	Joback Method
hfus	57.94	kJ/mol	Joback Method
hvap	93.34	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.690		Crippen Method
mcvol	346.010	ml/mol	McGowan Method
pc	1010.37	kPa	Joback Method
rinpol	3543.00		NIST Webbook
rinpol	3543.00		NIST Webbook
tb	960.16	K	Joback Method
tc	1175.51	K	Joback Method
tf	578.25	K	Joback Method
vc	1.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1148.50	J/mol×K	960.16	Joback Method
cpg	1164.75	J/mol×K	996.05	Joback Method
cpg	1179.44	J/mol×K	1031.94	Joback Method
cpg	1192.59	J/mol×K	1067.83	Joback Method
cpg	1204.21	J/mol×K	1103.72	Joback Method
cpg	1214.32	J/mol×K	1139.61	Joback Method
cpg	1222.95	J/mol×K	1175.51	Joback Method
dvisc	0.0002350	Pa×s	578.25	Joback Method

dvisc	0.0001321	Pa×s	641.90	Joback Method
dvisc	0.0000824	Pa×s	705.55	Joback Method
dvisc	0.0000555	Pa×s	769.21	Joback Method
dvisc	0.0000398	Pa×s	832.86	Joback Method
dvisc	0.0000299	Pa×s	896.51	Joback Method
dvisc	0.0000233	Pa×s	960.16	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=U382713&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