Diglycolic acid, 2,5-dimethylphenyl hexyl ester

Inchi: InChI=1S/C18H26O5/c1-4-5-6-7-10-22-17(19)12-21-13-18(20)23-16-11-14(2)8-9-15(16)3

InchiKey: HZTFCUMIWAZXOY-UHFFFAOYSA-N

Formula: C18H26O5

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

Mol. weight [g/mol]: 322.40

Physical Properties

Property code	Value	Unit	Source
gf	-379.01	kJ/mol	Joback Method
hf	-823.08	kJ/mol	Joback Method
hfus	42.40	kJ/mol	Joback Method
hvap	79.98	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.349		Crippen Method
mcvol	261.470	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	2828.00		NIST Webbook
rinpol	2828.00		NIST Webbook
tb	822.88	K	Joback Method
tc	1023.72	K	Joback Method
tf	510.63	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.23	J/mol×K	822.88	Joback Method
cpg	804.38	J/mol×K	856.35	Joback Method
cpg	818.44	J/mol×K	889.83	Joback Method
cpg	831.39	J/mol×K	923.30	Joback Method
cpg	843.23	J/mol×K	956.78	Joback Method
cpg	853.98	J/mol×K	990.25	Joback Method
cpg	863.61	J/mol×K	1023.72	Joback Method
dvisc	0.0004391	Pa×s	510.63	Joback Method

dvisc	0.0002647	Pa×s	562.67	Joback Method
dvisc	0.0001738	Pa×s	614.71	Joback Method
dvisc	0.0001219	Pa×s	666.75	Joback Method
dvisc	0.0000900	Pa×s	718.80	Joback Method
dvisc	0.0000692	Pa×s	770.84	Joback Method
dvisc	0.0000550	Pa×s	822.88	Joback Method

Sources

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=U382708&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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