

Diglycolic acid, 2-methylphenyl undecyl ester

Inchi:	InChI=1S/C22H34O5/c1-3-4-5-6-7-8-9-10-13-16-26-21(23)17-25-18-22(24)27-20-15-12-
InchiKey:	XAMRFQXYXKYHSM-UHFFFAOYSA-N
Formula:	C22H34O5
SMILES:	CCCCCCCCCOC(=O)COCC(=O)Oc1ccccc1C
Mol. weight [g/mol]:	378.50

Physical Properties

Property code	Value	Unit	Source
gf	-335.70	kJ/mol	Joback Method
hf	-894.17	kJ/mol	Joback Method
hfus	53.15	kJ/mol	Joback Method
hvap	88.23	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.991		Crippen Method
mvol	317.830	ml/mol	McGowan Method
pc	1157.71	kPa	Joback Method
rinpol	3522.00		NIST Webbook
rinpol	3522.00		NIST Webbook
tb	909.42	K	Joback Method
tc	1115.54	K	Joback Method
tf	543.19	K	Joback Method
vc	1.226	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.01	J/molxK	909.42	Joback Method
cpg	1043.01	J/molxK	943.77	Joback Method
cpg	1057.67	J/molxK	978.13	Joback Method
cpg	1070.99	J/molxK	1012.48	Joback Method
cpg	1082.99	J/molxK	1046.83	Joback Method
cpg	1093.70	J/molxK	1081.18	Joback Method
cpg	1103.12	J/molxK	1115.54	Joback Method
dvisc	0.0003352	Paxs	543.19	Joback Method

dvisc	0.0001841	Paxs	604.23	Joback Method
dvisc	0.0001129	Paxs	665.27	Joback Method
dvisc	0.0000751	Paxs	726.31	Joback Method
dvisc	0.0000532	Paxs	787.34	Joback Method
dvisc	0.0000397	Paxs	848.38	Joback Method
dvisc	0.0000307	Paxs	909.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U382013&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

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

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