Terephthalic acid, 3-hexyl tridecyl ester

Inchi: InChI=1S/C27H44O4/c1-4-7-8-9-10-11-12-13-14-15-16-22-30-26(28)23-18-20-24(21-19-
InchiKey: XLNDIJGFLUQSHJ-UHFFFAOYSA-N
Formula: C27H44O4
SMILES: CCCCCCCCCCCCCOC(=O)c1ccc(C(=O)OC(CC)CCC)cc1
Mol. weight [g/mol]: 432.64

Physical Properties

Property code	Value	Unit	Source
gf	-191.04	kJ/mol	Joback Method
hf	-870.43	kJ/mol	Joback Method
hfus	61.39	kJ/mol	Joback Method
hvap	96.56	kJ/mol	Joback Method
log10ws	-9.18		Crippen Method
logp	7.890		Crippen Method
mcvol	382.410	ml/mol	McGowan Method
pc	868.11	kPa	Joback Method
rinpol	3085.00		NIST Webbook
rinpol	3085.00		NIST Webbook
tb	1000.96	K	Joback Method
tc	1226.87	K	Joback Method
tf	562.31	K	Joback Method
vc	1.482	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1306.77	J/mol×K	1000.96	Joback Method
cpg	1324.54	J/mol×K	1038.61	Joback Method
cpg	1340.65	J/mol×K	1076.26	Joback Method
cpg	1355.17	J/mol×K	1113.92	Joback Method
cpg	1368.14	J/mol×K	1151.57	Joback Method
cpg	1379.63	J/mol×K	1189.22	Joback Method
cpg	1389.70	J/mol×K	1226.87	Joback Method
dvisc	0.0002962	Pa×s	562.31	Joback Method

dvisc	0.0001415	Pa×s	635.42	Joback Method
dvisc	0.0000788	Pa×s	708.53	Joback Method
dvisc	0.0000489	Pa×s	781.63	Joback Method
dvisc	0.0000330	Pa×s	854.74	Joback Method
dvisc	0.0000236	Pa×s	927.85	Joback Method
dvisc	0.0000178	Pa×s	1000.96	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=U356236&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

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