Isophthalic acid, cis-hex-3-enyl tridecyl ester

Inchi: InChI=1S/C27H42O4/c1-3-5-7-9-10-11-12-13-14-15-17-22-31-27(29)25-20-18-19-24(23-
InchiKey: BCGNUKOOZBNALI-VURMDHGXSA-N
Formula: C27H42O4
SMILES: CCC=CCCOC(=O)c1cccc(C(=O)OCCCCCCCCCCCCCC)c1
Mol. weight [g/mol]: 430.62

Physical Properties

Property code	Value	Unit	Source
gf	-108.38	kJ/mol	Joback Method
hf	-747.93	kJ/mol	Joback Method
hfus	65.11	kJ/mol	Joback Method
hvap	96.90	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	7.668		Crippen Method
mcvol	378.110	ml/mol	McGowan Method
pc	891.07	kPa	Joback Method
rinpol	3150.00		NIST Webbook
tb	1005.56	K	Joback Method
tc	1232.11	K	Joback Method
tf	572.23	K	Joback Method
vc	1.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1277.89	J/mol×K	1005.56	Joback Method
cpg	1352.04	J/mol×K	1194.35	Joback Method
cpg	1339.83	J/mol×K	1156.59	Joback Method
cpg	1326.39	J/mol×K	1118.83	Joback Method
cpg	1311.64	J/mol×K	1081.08	Joback Method
cpg	1295.50	J/mol×K	1043.32	Joback Method
cpg	1363.08	J/mol×K	1232.11	Joback Method
dvisc	0.0000172	Pa×s	1005.56	Joback Method
dvisc	0.0000226	Pa×s	933.34	Joback Method

dvisc	0.0000311	Pa×s	861.12	Joback Method
dvisc	0.0000453	Pa×s	788.89	Joback Method
dvisc	0.0000712	Pa×s	716.67	Joback Method
dvisc	0.0001241	Pa×s	644.45	Joback Method
dvisc	0.0002485	Pa×s	572.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356707&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