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

Inchi: InChI=1S/C28H44O4/c1-3-5-7-9-10-11-12-13-14-15-16-18-23-32-28(30)26-21-19-20-25(

InchiKey: LPEXOTIFECGJQD-VURMDHGXSA-N

Formula: C28H44O4

SMILES: CCC=CCCOC(=O)c1cccc(C(=O)OCCCCCCCCCCCCCCC)c1

Mol. weight [g/mol]: 444.65

Physical Properties

Property code	Value	Unit	Source
gf	-99.96	kJ/mol	Joback Method
hf	-768.57	kJ/mol	Joback Method
hfus	67.70	kJ/mol	Joback Method
hvap	99.13	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.058		Crippen Method
mcvol	392.200	ml/mol	McGowan Method
pc	842.11	kPa	Joback Method
rinpol	3251.00		NIST Webbook
tb	1028.44	K	Joback Method
tc	1262.21	K	Joback Method
tf	583.50	K	Joback Method
vc	1.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1340.94	J/mol×K	1028.44	Joback Method
cpg	1358.94	J/mol×K	1067.40	Joback Method
cpg	1375.39	J/mol×K	1106.36	Joback Method
cpg	1390.37	J/mol×K	1145.33	Joback Method
cpg	1403.97	J/mol×K	1184.29	Joback Method
cpg	1416.27	J/mol×K	1223.25	Joback Method
cpg	1427.36	J/mol×K	1262.21	Joback Method
dvisc	0.0002193	Pa×s	583.50	Joback Method
dvisc	0.0001085	Pa×s	657.66	Joback Method

dvisc	0.0000619	Pa×s	731.81	Joback Method
dvisc	0.0000392	Pa×s	805.97	Joback Method
dvisc	0.0000268	Pa×s	880.13	Joback Method
dvisc	0.0000194	Pa×s	954.28	Joback Method
dvisc	0.0000147	Pa×s	1028.44	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=U356708&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