Isophthalic acid, cis-tetradec-3-enyl nonyl ester

Inchi: InChI=1S/C31H50O4/c1-3-5-7-9-11-12-13-14-15-17-19-21-26-35-31(33)29-24-22-23-28(

InchiKey: FVMUDWKWMAIOAO-ZPHPHTNESA-N

Formula: C31H50O4

SMILES: CCCCCCCCCCC=CCCOC(=O)c1cccc(C(=O)OCCCCCCCCCC)c1

Mol. weight [g/mol]: 486.73

Physical Properties

Property code	Value	Unit	Source
gf	-74.70	kJ/mol	Joback Method
hf	-830.49	kJ/mol	Joback Method
hfus	75.47	kJ/mol	Joback Method
hvap	105.81	kJ/mol	Joback Method
log10ws	-10.60		Crippen Method
logp	9.228		Crippen Method
mcvol	434.470	ml/mol	McGowan Method
pc	717.22	kPa	Joback Method
rinpol	3558.00		NIST Webbook
tb	1097.08	K	Joback Method
tc	1360.33	K	Joback Method
tf	617.31	K	Joback Method
vc	1.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1532.26	J/mol×K	1097.08	Joback Method
cpg	1551.78	J/mol×K	1140.95	Joback Method
cpg	1569.37	J/mol×K	1184.83	Joback Method
cpg	1585.18	J/mol×K	1228.70	Joback Method
cpg	1599.35	J/mol×K	1272.58	Joback Method
cpg	1612.02	J/mol×K	1316.45	Joback Method
cpg	1623.33	J/mol×K	1360.33	Joback Method
dvisc	0.0001483	Pa×s	617.31	Joback Method
dvisc	0.0000716	Pa×s	697.27	Joback Method

dvisc	0.0000401	Pa×s	777.23	Joback Method
dvisc	0.0000250	Pa×s	857.19	Joback Method
dvisc	0.0000169	Pa×s	937.16	Joback Method
dvisc	0.0000122	Pa×s	1017.12	Joback Method
dvisc	0.0000092	Pa×s	1097.08	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=U356735&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