Phthalic acid, cis-hex-3-enyl heptadecyl ester

Inchi: InChI=1S/C31H50O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-23-27-35-31(33)29-25-
InchiKey: AGBKYFGFFHAYER-VURMDHGXSA-N
Formula: C31H50O4
SMILES: CCC=CCCOC(=O)c1ccccc1C(=O)OCCCCCCCCCCCCCCCCC
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	3457.00		NIST Webbook
rinpol	3457.00		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=U360421&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