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

Inchi: InChI=1S/C32H52O4/c1-3-5-7-9-10-11-12-13-14-15-16-17-18-19-20-24-28-36-32(34)30-
InchiKey: YAPKMXPAPDIWEF-VURMDHGXSA-N
Formula: C32H52O4
SMILES: CCC=CCCOC(=O)c1ccccc1C(=O)OCCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 500.75

Physical Properties

Property code	Value	Unit	Source
gf	-66.28	kJ/mol	Joback Method
hf	-851.13	kJ/mol	Joback Method
hfus	78.06	kJ/mol	Joback Method
hvap	108.03	kJ/mol	Joback Method
log10ws	-11.02		Crippen Method
logp	9.618		Crippen Method
mcvol	448.560	ml/mol	McGowan Method
pc	681.71	kPa	Joback Method
rinpol	3572.00		NIST Webbook
tb	1119.96	K	Joback Method
tc	1395.96	K	Joback Method
tf	628.58	K	Joback Method
vc	1.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1596.66	J/mol×K	1119.96	Joback Method
cpg	1616.80	J/mol×K	1165.96	Joback Method
cpg	1634.86	J/mol×K	1211.96	Joback Method
cpg	1651.01	J/mol×K	1257.96	Joback Method
cpg	1665.42	J/mol×K	1303.96	Joback Method
cpg	1678.25	J/mol×K	1349.96	Joback Method
cpg	1689.69	J/mol×K	1395.96	Joback Method
dvisc	0.0001296	Pa×s	628.58	Joback Method
dvisc	0.0000620	Pa×s	710.48	Joback Method

dvisc	0.0000346	Pa×s	792.37	Joback Method
dvisc	0.0000215	Pa×s	874.27	Joback Method
dvisc	0.0000145	Pa×s	956.17	Joback Method
dvisc	0.0000104	Pa×s	1038.06	Joback Method
dvisc	0.0000078	Pa×s	1119.96	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=U360447&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