

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)c1cccc1C(=O)OCCCCCCCCCCCCCCCC
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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1532.26	J/molxK	1097.08	Joback Method
cpg	1551.78	J/molxK	1140.95	Joback Method
cpg	1569.37	J/molxK	1184.83	Joback Method
cpg	1585.18	J/molxK	1228.70	Joback Method
cpg	1599.35	J/molxK	1272.58	Joback Method
cpg	1612.02	J/molxK	1316.45	Joback Method
cpg	1623.33	J/molxK	1360.33	Joback Method
dvisc	0.0001483	Paxs	617.31	Joback Method

dvisc	0.0000716	Paxs	697.27	Joback Method
dvisc	0.0000401	Paxs	777.23	Joback Method
dvisc	0.0000250	Paxs	857.19	Joback Method
dvisc	0.0000169	Paxs	937.16	Joback Method
dvisc	0.0000122	Paxs	1017.12	Joback Method
dvisc	0.0000092	Paxs	1097.08	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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