

Phthalic acid, 6-methylhept-2-yl octadecyl ester

Inchi:	InChI=1S/C34H58O4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-22-28-37-33(35)31-2
InchiKey:	BGIHRDUVCMHKKB-UHFFFAOYSA-N
Formula:	C34H58O4
SMILES:	CCCCCCCCCCCCCCCCCOC(=O)c1cccc1C(=O)OC(C)CCCC(C)C
Mol. weight [g/mol]:	530.82

Physical Properties

Property code	Value	Unit	Source
gf	-134.54	kJ/mol	Joback Method
hf	-1020.19	kJ/mol	Joback Method
hfus	76.00	kJ/mol	Joback Method
hvap	111.75	kJ/mol	Joback Method
log10ws	-11.87		Crippen Method
logp	10.476		Crippen Method
mcvol	481.040	ml/mol	McGowan Method
pc	607.26	kPa	Joback Method
rinpol	3616.00		NIST Webbook
tb	1160.68	K	Joback Method
tc	1464.46	K	Joback Method
tf	626.20	K	Joback Method
vc	1.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1753.89	J/molxK	1160.68	Joback Method
cpg	1774.09	J/molxK	1211.31	Joback Method
cpg	1791.35	J/molxK	1261.94	Joback Method
cpg	1805.88	J/molxK	1312.57	Joback Method
cpg	1817.90	J/molxK	1363.20	Joback Method
cpg	1827.59	J/molxK	1413.83	Joback Method
cpg	1835.17	J/molxK	1464.46	Joback Method
dvisc	0.0001248	Paxs	626.20	Joback Method
dvisc	0.0000530	Paxs	715.28	Joback Method

dvisc	0.0000272	Paxs	804.36	Joback Method
dvisc	0.0000160	Paxs	893.44	Joback Method
dvisc	0.0000103	Paxs	982.52	Joback Method
dvisc	0.0000072	Paxs	1071.60	Joback Method
dvisc	0.0000053	Paxs	1160.68	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U377972&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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