Phthalic acid, 4-methylhept-3-yl octadecyl ester

Inchi: InChI=1S/C34H58O4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-28-37-33(35)30
InchiKey: SWUWXTWUVYOZLV-UHFFFAOYSA-N
Formula: C34H58O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(CC)C(C)CCC
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	3602.00		NIST Webbook
rinpol	3602.00		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/mol×K	1160.68	Joback Method
cpg	1774.09	J/mol×K	1211.31	Joback Method
cpg	1791.35	J/mol×K	1261.94	Joback Method
cpg	1805.88	J/mol×K	1312.57	Joback Method
cpg	1817.90	J/mol×K	1363.20	Joback Method
cpg	1827.59	J/mol×K	1413.83	Joback Method
cpg	1835.17	J/mol×K	1464.46	Joback Method
dvisc	0.0001248	Pa×s	626.20	Joback Method

dvisc	0.0000530	Pa×s	715.28	Joback Method
dvisc	0.0000272	Pa×s	804.36	Joback Method
dvisc	0.0000160	Pa×s	893.44	Joback Method
dvisc	0.0000103	Pa×s	982.52	Joback Method
dvisc	0.0000072	Pa×s	1071.60	Joback Method
dvisc	0.0000053	Pa×s	1160.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377953&Units=SI
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

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