Phthalic acid, octadecyl 2-propylpentyl ester

Inchi: InChI=1S/C34H58O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-28-37-33(35)31-
InchiKey: CWDXYOBIFBTGBI-UHFFFAOYSA-N
Formula: C34H58O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(CCC)CCC
Mol. weight [g/mol]: 530.82

Physical Properties

Property code	Value	Unit	Source
gf	-132.10	kJ/mol	Joback Method
hf	-1014.91	kJ/mol	Joback Method
hfus	79.52	kJ/mol	Joback Method
hvap	112.14	kJ/mol	Joback Method
log10ws	-11.76		Crippen Method
logp	10.478		Crippen Method
mcvol	481.040	ml/mol	McGowan Method
pc	604.87	kPa	Joback Method
rinpol	3645.00		NIST Webbook
tb	1161.12	K	Joback Method
tc	1469.33	K	Joback Method
tf	641.20	K	Joback Method
vc	1.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1753.98	J/mol×K	1161.12	Joback Method
cpg	1774.62	J/mol×K	1212.49	Joback Method
cpg	1792.27	J/mol×K	1263.86	Joback Method
cpg	1807.14	J/mol×K	1315.23	Joback Method
cpg	1819.46	J/mol×K	1366.59	Joback Method
cpg	1829.43	J/mol×K	1417.96	Joback Method
cpg	1837.28	J/mol×K	1469.33	Joback Method
dvisc	0.0001145	Pa×s	641.20	Joback Method
dvisc	0.0000519	Pa×s	727.85	Joback Method

dvisc	0.0000278	Pa×s	814.51	Joback Method
dvisc	0.0000168	Pa×s	901.16	Joback Method
dvisc	0.0000111	Pa×s	987.81	Joback Method
dvisc	0.0000078	Pa×s	1074.47	Joback Method
dvisc	0.0000058	Pa×s	1161.12	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=U377934&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