Phthalic acid, heptadecyl 2-propylpentyl ester

Inchi: InChI=1S/C33H56O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-22-27-36-32(34)30-25-
InchiKey: DKGWALOUTUVALT-UHFFFAOYSA-N
Formula: C33H56O4
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(CCC)CCC
Mol. weight [g/mol]: 516.80

Physical Properties

Property code	Value	Unit	Source
gf	-140.52	kJ/mol	Joback Method
hf	-994.27	kJ/mol	Joback Method
hfus	76.93	kJ/mol	Joback Method
hvap	109.91	kJ/mol	Joback Method
log10ws	-11.34		Crippen Method
logp	10.088		Crippen Method
mcvol	466.950	ml/mol	McGowan Method
pc	634.48	kPa	Joback Method
rinpol	3543.00		NIST Webbook
rinpol	3543.00		NIST Webbook
tb	1138.24	K	Joback Method
tc	1429.88	K	Joback Method
tf	629.93	K	Joback Method
vc	1.817	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1689.47	J/mol×K	1138.24	Joback Method
cpg	1709.60	J/mol×K	1186.85	Joback Method
cpg	1727.00	J/mol×K	1235.45	Joback Method
cpg	1741.86	J/mol×K	1284.06	Joback Method
cpg	1754.36	J/mol×K	1332.66	Joback Method
cpg	1764.66	J/mol×K	1381.27	Joback Method
cpg	1772.94	J/mol×K	1429.88	Joback Method
dvisc	0.0001320	Pa×s	629.93	Joback Method

dvisc	0.0000602	Pa×s	714.65	Joback Method
dvisc	0.0000324	Pa×s	799.37	Joback Method
dvisc	0.0000196	Pa×s	884.08	Joback Method
dvisc	0.0000130	Pa×s	968.80	Joback Method
dvisc	0.0000092	Pa×s	1053.52	Joback Method
dvisc	0.0000068	Pa×s	1138.24	Joback Method

Sources

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=U377933&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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