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

Inchi: InChI=1S/C33H56O4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-23-27-36-32(34)29-25

InchiKey: XCOMBEJEBSJORI-UHFFFAOYSA-N

Formula: C33H56O4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(CC)C(C)CCC

Mol. weight [g/mol]: 516.80

Physical Properties

Property code	Value	Unit	Source
gf	-142.96	kJ/mol	Joback Method
hf	-999.55	kJ/mol	Joback Method
hfus	73.41	kJ/mol	Joback Method
hvap	109.53	kJ/mol	Joback Method
log10ws	-11.45		Crippen Method
logp	10.086		Crippen Method
mcvol	466.950	ml/mol	McGowan Method
pc	637.05	kPa	Joback Method
rinpol	3501.00		NIST Webbook
rinpol	3501.00		NIST Webbook
tb	1137.80	K	Joback Method
tc	1425.65	K	Joback Method
tf	614.93	K	Joback Method
vc	1.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1689.45	J/mol×K	1137.80	Joback Method
cpg	1763.06	J/mol×K	1377.68	Joback Method
cpg	1753.01	J/mol×K	1329.70	Joback Method
cpg	1740.80	J/mol×K	1281.73	Joback Method
cpg	1726.25	J/mol×K	1233.75	Joback Method
cpg	1709.19	J/mol×K	1185.78	Joback Method
cpg	1771.10	J/mol×K	1425.65	Joback Method
dvisc	0.0000062	Pa×s	1137.80	Joback Method

dvisc	0.0000084	Pa×s	1050.65	Joback Method
dvisc	0.0000121	Pa×s	963.51	Joback Method
dvisc	0.0000187	Pa×s	876.37	Joback Method
dvisc	0.0000318	Pa×s	789.22	Joback Method
dvisc	0.0000617	Pa×s	702.08	Joback Method
dvisc	0.0001443	Pa×s	614.93	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=U377952&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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