Phthalic acid, hexadecyl 2-methylbenzyl ester

Inchi: InChI=1S/C32H46O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-20-25-35-31(33)29-23-18-19-2
InchiKey: RZSOXFATAWPBPH-UHFFFAOYSA-N
Formula: C32H46O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccccc1C
Mol. weight [g/mol]: 494.71

Physical Properties

Property code	Value	Unit	Source
gf	-43.72	kJ/mol	Joback Method
hf	-743.29	kJ/mol	Joback Method
hfus	71.51	kJ/mol	Joback Method
hvap	111.01	kJ/mol	Joback Method
log10ws	-10.82		Crippen Method
logp	8.990		Crippen Method
mcvol	429.100	ml/mol	McGowan Method
pc	786.39	kPa	Joback Method
rinpol	3565.00		NIST Webbook
rinpol	3565.00		NIST Webbook
tb	1147.46	K	Joback Method
tc	1416.05	K	Joback Method
tf	672.60	K	Joback Method
vc	1.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1508.60	J/mol×K	1147.46	Joback Method
cpg	1523.83	J/mol×K	1192.22	Joback Method
cpg	1536.99	J/mol×K	1236.99	Joback Method
cpg	1548.22	J/mol×K	1281.75	Joback Method
cpg	1557.64	J/mol×K	1326.52	Joback Method
cpg	1565.38	J/mol×K	1371.28	Joback Method
cpg	1571.57	J/mol×K	1416.05	Joback Method
dvisc	0.0001143	Pa×s	672.60	Joback Method

dvisc	0.0000609	Pa×s	751.74	Joback Method
dvisc	0.0000366	Pa×s	830.89	Joback Method
dvisc	0.0000240	Pa×s	910.03	Joback Method
dvisc	0.0000168	Pa×s	989.17	Joback Method
dvisc	0.0000125	Pa×s	1068.32	Joback Method
dvisc	0.0000096	Pa×s	1147.46	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=U382862&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