Phthalic acid, 2,4-dichlorobenzyl tridecyl ester

Inchi: InChI=1S/C28H36Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-14-19-33-27(31)24-15-12-13-16-25(24
InchiKey: PTXCKIVRSGPSGW-UHFFFAOYSA-N
Formula: C28H36Cl2O4
SMILES: CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 507.49

Physical Properties

Property code	Value	Unit	Source
gf	-110.89	kJ/mol	Joback Method
hf	-703.68	kJ/mol	Joback Method
hfus	69.16	kJ/mol	Joback Method
hvap	111.54	kJ/mol	Joback Method
log10ws	-10.46		Crippen Method
logp	8.818		Crippen Method
mcvol	397.220	ml/mol	McGowan Method
pc	934.63	kPa	Joback Method
rinpol	3492.00		NIST Webbook
rinpol	3492.00		NIST Webbook
tb	1135.78	K	Joback Method
tc	1392.82	K	Joback Method
tf	699.88	K	Joback Method
vc	1.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1298.93	J/mol×K	1135.78	Joback Method
cpg	1340.93	J/mol×K	1349.98	Joback Method
cpg	1335.66	J/mol×K	1307.14	Joback Method
cpg	1328.92	J/mol×K	1264.30	Joback Method
cpg	1320.61	J/mol×K	1221.46	Joback Method
cpg	1310.64	J/mol×K	1178.62	Joback Method
cpg	1344.81	J/mol×K	1392.82	Joback Method
dvisc	0.0000128	Pa×s	1135.78	Joback Method

dvisc	0.0000163	Pa×s	1063.13	Joback Method
dvisc	0.0000213	Pa×s	990.48	Joback Method
dvisc	0.0000292	Pa×s	917.83	Joback Method
dvisc	0.0000423	Pa×s	845.18	Joback Method
dvisc	0.0000655	Pa×s	772.53	Joback Method
dvisc	0.0001112	Pa×s	699.88	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=U382568&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