

Phthalic acid, 2-chloropropyl hexadecyl ester

Inchi:	InChI=1S/C27H43ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-31-26(29)24-19-16-17
InchiKey:	SAJLQJCDWMVHK-UHFFFAOYSA-N
Formula:	C27H43ClO4
SMILES:	CCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCC(C)Cl
Mol. weight [g/mol]:	467.08

Physical Properties

Property code	Value	Unit	Source
gf	-202.97	kJ/mol	Joback Method
hf	-886.17	kJ/mol	Joback Method
hfus	65.59	kJ/mol	Joback Method
hvap	100.94	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	8.109		Crippen Method
mvol	394.650	ml/mol	McGowan Method
pc	849.49	kPa	Joback Method
rinpol	3274.00		NIST Webbook
rinpol	3274.00		NIST Webbook
tb	1038.39	K	Joback Method
tc	1274.58	K	Joback Method
tf	592.23	K	Joback Method
vc	1.530	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1332.45	J/molxK	1038.39	Joback Method
cpg	1349.03	J/molxK	1077.76	Joback Method
cpg	1363.88	J/molxK	1117.12	Joback Method
cpg	1377.09	J/molxK	1156.49	Joback Method
cpg	1388.73	J/molxK	1195.85	Joback Method
cpg	1398.85	J/molxK	1235.22	Joback Method
cpg	1407.54	J/molxK	1274.58	Joback Method
dvisc	0.0002302	Paxs	592.23	Joback Method

dvisc	0.0001129	Paxs	666.59	Joback Method
dvisc	0.0000639	Paxs	740.95	Joback Method
dvisc	0.0000401	Paxs	815.31	Joback Method
dvisc	0.0000272	Paxs	889.67	Joback Method
dvisc	0.0000196	Paxs	964.03	Joback Method
dvisc	0.0000148	Paxs	1038.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U356837&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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