

2-Chlorobenzoic acid, 3-pentadecyl ester

Inchi:	InChI=1S/C22H35ClO2/c1-3-5-6-7-8-9-10-11-12-13-16-19(4-2)25-22(24)20-17-14-15-18
InchiKey:	LIPZCBXPWHSJGI-UHFFFAOYSA-N
Formula:	C22H35ClO2
SMILES:	CCCCCCCCCCCC(CC)OC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	366.96

Physical Properties

Property code	Value	Unit	Source
gf	-11.15	kJ/mol	Joback Method
hf	-538.17	kJ/mol	Joback Method
hfus	49.85	kJ/mol	Joback Method
hvap	80.66	kJ/mol	Joback Method
log10ws	-8.37		Crippen Method
logp	7.586		Crippen Method
mvol	316.760	ml/mol	McGowan Method
pc	1113.34	kPa	Joback Method
rinpol	2516.00		NIST Webbook
rinpol	2516.00		NIST Webbook
tb	847.70	K	Joback Method
tc	1046.95	K	Joback Method
tf	463.72	K	Joback Method
vc	1.226	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	976.83	J/molxK	847.70	Joback Method
cpg	994.55	J/molxK	880.91	Joback Method
cpg	1011.14	J/molxK	914.12	Joback Method
cpg	1026.64	J/molxK	947.33	Joback Method
cpg	1041.09	J/molxK	980.54	Joback Method
cpg	1054.54	J/molxK	1013.74	Joback Method
cpg	1067.03	J/molxK	1046.95	Joback Method
dvisc	0.0008036	Paxs	463.72	Joback Method

dvisc	0.0003724	Paxs	527.72	Joback Method
dvisc	0.0002038	Paxs	591.71	Joback Method
dvisc	0.0001254	Paxs	655.71	Joback Method
dvisc	0.0000842	Paxs	719.71	Joback Method
dvisc	0.0000603	Paxs	783.70	Joback Method
dvisc	0.0000454	Paxs	847.70	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=U299822&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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