2-Chlorobenzoic acid, 8-pentadecyl ester

Inchi: InChI=1S/C22H35ClO2/c1-3-5-7-9-11-15-19(16-12-10-8-6-4-2)25-22(24)20-17-13-14-18-
InchiKey: NFAWPWNROYXQCJ-UHFFFAOYSA-N
Formula: C22H35ClO2
SMILES: CCCCCCCC(CCCCCCC)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
mcvol	316.760	ml/mol	McGowan Method
pc	1113.34	kPa	Joback Method
rinpol	2460.00		NIST Webbook
rinpol	2460.00		NIST Webbook
tb	847.70	K	Joback Method
tc	1046.95	K	Joback Method
tf	463.72	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0003724	Pa×s	527.72	Joback Method
dvisc	0.0002038	Pa×s	591.71	Joback Method
dvisc	0.0001254	Pa×s	655.71	Joback Method
dvisc	0.0000842	Pa×s	719.71	Joback Method
dvisc	0.0000603	Pa×s	783.70	Joback Method
dvisc	0.0000454	Pa×s	847.70	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=U299827&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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