3-Chloro-2-fluorobenzoic acid, 6-chlorohexyl ester

Inchi: InChI=1S/C13H15Cl2FO2/c14-8-3-1-2-4-9-18-13(17)10-6-5-7-11(15)12(10)16/h5-7H,1-4,
InchiKey: DEMDOORCUCINHP-UHFFFAOYSA-N
Formula: C13H15Cl2FO2
SMILES: O=C(OCCCCCCCl)c1cccc(Cl)c1F
Mol. weight [g/mol]: 293.16

Physical Properties

Property code	Value	Unit	Source
gf	-300.86	kJ/mol	Joback Method
hf	-570.45	kJ/mol	Joback Method
hfus	36.95	kJ/mol	Joback Method
hvap	65.24	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.435		Crippen Method
mcvol	203.960	ml/mol	McGowan Method
pc	1996.55	kPa	Joback Method
rinpol	2105.00		NIST Webbook
tb	683.90	K	Joback Method
tc	887.36	K	Joback Method
tf	420.32	K	Joback Method
vc	0.795	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.01	J/mol×K	683.90	Joback Method
cpg	517.88	J/mol×K	717.81	Joback Method
cpg	529.97	J/mol×K	751.72	Joback Method
cpg	541.29	J/mol×K	785.63	Joback Method
cpg	551.88	J/mol×K	819.54	Joback Method
cpg	561.75	J/mol×K	853.45	Joback Method
cpg	570.91	J/mol×K	887.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357331&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
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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