3-Chloro-2-fluorobenzoic acid, dodecyl ester

Other names: 3-Chloro-2-fluorobenzoic acid, dodceyl ester
Inchi: InChI=1S/C19H28ClFO2/c1-2-3-4-5-6-7-8-9-10-11-15-23-19(22)16-13-12-14-17(20)18(1
InchiKey: MUKSKSBEVNLRGR-UHFFFAOYSA-N
Formula: C19H28ClFO2
SMILES: CCCCCCCCCCCCOC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]: 342.88

Physical Properties

Property code	Value	Unit	Source
gf	-238.41	kJ/mol	Joback Method
hf	-678.55	kJ/mol	Joback Method
hfus	48.29	kJ/mol	Joback Method
hvap	74.21	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	6.557		Crippen Method
mcvol	276.260	ml/mol	McGowan Method
pc	1296.73	kPa	Joback Method
rinpol	2417.00		NIST Webbook
rinpol	2417.00		NIST Webbook
tb	783.75	K	Joback Method
tc	975.77	K	Joback Method
tf	458.02	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.84	J/mol×K	783.75	Joback Method
cpg	822.09	J/mol×K	815.75	Joback Method
cpg	837.37	J/mol×K	847.76	Joback Method
cpg	851.72	J/mol×K	879.76	Joback Method
cpg	865.18	J/mol×K	911.76	Joback Method
cpg	877.75	J/mol×K	943.77	Joback Method
cpg	889.48	J/mol×K	975.77	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=U338889&Units=SI

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