

3-Chloro2-fluorobenzoic acid, 5-tetradecyl ester

Inchi:	InChI=1S/C21H32ClFO2/c1-3-5-7-8-9-10-11-14-17(13-6-4-2)25-21(24)18-15-12-16-19(2)
InchiKey:	VMJQOEAEENSHLNT-UHFFFAOYSA-N
Formula:	C21H32ClFO2
SMILES:	CCCCCCCCC(CCCC)OC(=O)c1cccc(Cl)c1F
Mol. weight [g/mol]:	370.93

Physical Properties

Property code	Value	Unit	Source
gf	-224.01	kJ/mol	Joback Method
hf	-725.11	kJ/mol	Joback Method
hfus	49.95	kJ/mol	Joback Method
hvap	78.28	kJ/mol	Joback Method
log10ws	-8.28		Crippen Method
logp	7.335		Crippen Method
mcvol	304.440	ml/mol	McGowan Method
pc	1140.57	kPa	Joback Method
rinpol	2457.00		NIST Webbook
rinpol	2457.00		NIST Webbook
tb	829.07	K	Joback Method
tc	1024.31	K	Joback Method
tf	465.56	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	923.79	J/molxK	829.07	Joback Method
cpg	940.76	J/molxK	861.61	Joback Method
cpg	956.68	J/molxK	894.15	Joback Method
cpg	971.57	J/molxK	926.69	Joback Method
cpg	985.47	J/molxK	959.23	Joback Method
cpg	998.41	J/molxK	991.77	Joback Method
cpg	1010.42	J/molxK	1024.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338648&Units=SI
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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