3-Chloro2-fluorobenzoic acid, 3-hexadecyl ester

Inchi: InChI=1S/C23H36ClFO2/c1-3-5-6-7-8-9-10-11-12-13-14-16-19(4-2)27-23(26)20-17-15-18

InchiKey: LBSZBBPFLCGGTD-UHFFFAOYSA-N

Formula: C23H36ClFO2

SMILES: CCCCCCCCCCCCCC(CC)OC(=O)c1cccc(Cl)c1F

Mol. weight [g/mol]: 398.98

Physical Properties

Property code	Value	Unit	Source
gf	-207.17	kJ/mol	Joback Method
hf	-766.39	kJ/mol	Joback Method
hfus	55.13	kJ/mol	Joback Method
hvap	82.73	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	8.116		Crippen Method
mcvol	332.620	ml/mol	McGowan Method
pc	1005.89	kPa	Joback Method
rinpol	2702.00		NIST Webbook
rinpol	2702.00		NIST Webbook
tb	874.83	K	Joback Method
tc	1074.11	K	Joback Method
tf	488.10	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1044.42	J/mol×K	874.83	Joback Method
cpg	1061.98	J/mol×K	908.04	Joback Method
cpg	1078.38	J/mol×K	941.26	Joback Method
cpg	1093.68	J/mol×K	974.47	Joback Method
cpg	1107.91	J/mol×K	1007.68	Joback Method
cpg	1121.11	J/mol×K	1040.89	Joback Method
cpg	1133.33	J/mol×K	1074.11	Joback Method

Sources

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=U338654&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Latest version available from:
https://www.chemeo.com/cid/73-722-9/3-Chloro2-fluorobenzoic-acid-3-hexadecyl-ester.pdf
Generated by Cheméo on 2024-04-19 02:10:56.48737073 +0000 UTC m=+15781905.407948052.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.