3-Chloro-2-fluorobenzoic acid, 2,4-dichloronaphth-1-yl ester

Inchi: InChI=1S/C17H8Cl3FO2/c18-12-7-3-6-11(15(12)21)17(22)23-16-10-5-2-1-4-9(10)13(19)8

InchiKey: APQRHWOUYQVKNL-UHFFFAOYSA-N

Formula: C17H8Cl3FO2

SMILES: O=C(Oc1c(Cl)cc(Cl)c2ccccc12)c1cccc(Cl)c1F

Mol. weight [g/mol]: 369.60

Physical Properties

Property code	Value	Unit	Source
gf	-88.94	kJ/mol	Joback Method
hf	-275.56	kJ/mol	Joback Method
hfus	41.40	kJ/mol	Joback Method
hvap	84.43	kJ/mol	Joback Method
log10ws	-7.75		Crippen Method
logp	6.158		Crippen Method
mcvol	229.340	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	2815.00		NIST Webbook
tb	873.45	K	Joback Method
tc	1127.41	K	Joback Method
tf	592.00	K	Joback Method
vc	0.882	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	566.56	J/mol×K	873.45	Joback Method
cpg	576.19	J/mol×K	915.78	Joback Method
cpg	584.92	J/mol×K	958.10	Joback Method
cpg	592.82	J/mol×K	1000.43	Joback Method
cpg	599.96	J/mol×K	1042.76	Joback Method
cpg	606.43	J/mol×K	1085.08	Joback Method
cpg	612.29	J/mol×K	1127.41	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=U357337&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