1-Naphthaleneacetic acid, 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C18H12ClFO2/c19-15-9-4-10-16(20)18(15)22-17(21)11-13-7-3-6-12-5-1-2-8-14

InchiKey: UGLDIXOMFHNHGZ-UHFFFAOYSA-N

Formula: C18H12ClFO2

SMILES: O=C(Cc1cccc2ccccc12)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 314.74

Physical Properties

Property code	Value	Unit	Source
gf	-37.40	kJ/mol	Joback Method
hf	-241.78	kJ/mol	Joback Method
hfus	36.37	kJ/mol	Joback Method
hvap	76.56	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	4.780		Crippen Method
mcvol	218.950	ml/mol	McGowan Method
pc	2224.99	kPa	Joback Method
rinpol	2981.00		NIST Webbook
rinpol	2981.00		NIST Webbook
tb	811.51	K	Joback Method
tc	1055.73	K	Joback Method
tf	518.39	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.11	J/mol×K	811.51	Joback Method
cpg	596.65	J/mol×K	852.21	Joback Method
cpg	608.13	J/mol×K	892.92	Joback Method
cpg	618.63	J/mol×K	933.62	Joback Method
cpg	628.23	J/mol×K	974.33	Joback Method
cpg	637.03	J/mol×K	1015.03	Joback Method
cpg	645.11	J/mol×K	1055.73	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415050&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
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
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