2,6-Difluoro-3-methylbenzoic acid, 2,4-dichloronaphthyl-1 ester

Inchi: InChI=1S/C18H10Cl2F2O2/c1-9-6-7-14(21)15(16(9)22)18(23)24-17-11-5-3-2-4-10(11)12

InchiKey: KYTPUFMVSWTGHM-UHFFFAOYSA-N

Formula: C18H10Cl2F2O2

SMILES: Cc1ccc(F)c(C(=O)Oc2c(Cl)cc(Cl)c3ccccc23)c1F

Mol. weight [g/mol]: 367.17

Physical Properties

Property code	Value	Unit	Source
gf	-273.03	kJ/mol	Joback Method
hf	-488.04	kJ/mol	Joback Method
hfus	42.48	kJ/mol	Joback Method
hvap	82.12	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	5.952		Crippen Method
mcvol	232.960	ml/mol	McGowan Method
pc	1980.59	kPa	Joback Method
rinpol	2732.00		NIST Webbook
tb	863.15	K	Joback Method
tc	1102.59	K	Joback Method
tf	586.46	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	607.49	J/mol×K	863.15	Joback Method
cpg	618.07	J/mol×K	903.06	Joback Method
cpg	627.74	J/mol×K	942.96	Joback Method
cpg	636.56	J/mol×K	982.87	Joback Method
cpg	644.57	J/mol×K	1022.78	Joback Method
cpg	651.84	J/mol×K	1062.68	Joback Method
cpg	658.43	J/mol×K	1102.59	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=U343763&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