2,6-Difluoro-3-methylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester

Inchi: InChI=1S/C15H8Cl2F2O3/c1-7-2-3-11(18)12(13(7)19)15(21)22-14-8(6-20)4-9(16)5-10(14

InchiKey: CJXZCXDGEDBCGJ-UHFFFAOYSA-N

Formula: C15H8Cl2F2O3

SMILES: Cc1ccc(F)c(C(=O)Oc2c(Cl)cc(Cl)cc2C=O)c1F

Mol. weight [g/mol]: 345.12

Physical Properties

Property code	Value	Unit	Source
gf	-504.46	kJ/mol	Joback Method
hf	-702.77	kJ/mol	Joback Method
hfus	39.98	kJ/mol	Joback Method
hvap	80.52	kJ/mol	Joback Method
log10ws	-6.31		Crippen Method
logp	4.612		Crippen Method
mcvol	211.720	ml/mol	McGowan Method
pc	2204.15	kPa	Joback Method
rinpol	2343.00		NIST Webbook
tb	824.19	K	Joback Method
tc	1053.32	K	Joback Method
tf	561.95	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	530.85	J/mol×K	824.19	Joback Method
cpg	540.27	J/mol×K	862.38	Joback Method
cpg	548.79	J/mol×K	900.57	Joback Method
cpg	556.44	J/mol×K	938.75	Joback Method
cpg	563.21	J/mol×K	976.94	Joback Method
cpg	569.12	J/mol×K	1015.13	Joback Method
cpg	574.18	J/mol×K	1053.32	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=U343760&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