6-Fluoro-3-trifluoromethylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester

Other names: 6-Fluoro-3-trifluorobenzoic acid, 2-formyl-4,6-dichlorophenyl ester

Inchi: InChI=1S/C15H6Cl2F4O3/c16-9-3-7(6-22)13(11(17)5-9)24-14(23)10-4-8(15(19,20)21)1-2

InchiKey: QGPSCRLJYNDTSF-UHFFFAOYSA-N

Formula: C15H6Cl2F4O3

SMILES: O=Cc1cc(Cl)cc(Cl)c1OC(=O)c1cc(C(F)(F)F)ccc1F

Mol. weight [g/mol]: 381.11

Physical Properties

Property code	Value	Unit	Source
gf	-881.61	kJ/mol	Joback Method
hf	-1092.27	kJ/mol	Joback Method
hfus	39.12	kJ/mol	Joback Method
hvap	76.93	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	5.183		Crippen Method
mcvol	215.260	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	2120.00		NIST Webbook
rinpol	2120.00		NIST Webbook
tb	814.52	K	Joback Method
tc	1036.79	K	Joback Method
tf	553.03	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.01	J/mol×K	814.52	Joback Method
cpg	558.68	J/mol×K	851.56	Joback Method
cpg	566.53	J/mol×K	888.61	Joback Method
cpg	573.58	J/mol×K	925.65	Joback Method
cpg	579.89	J/mol×K	962.70	Joback Method
cpg	585.49	J/mol×K	999.74	Joback Method
cpg	590.44	J/mol×K	1036.79	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=U343790&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