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

Inchi: InChI=1S/C14H8Cl2F2O2/c1-7-2-5-11(17)12(13(7)18)14(19)20-8-3-4-9(15)10(16)6-8/h2-

InchiKey: KVIJWMIURLLPQR-UHFFFAOYSA-N

Formula: C14H8Cl2F2O2

SMILES: Cc1ccc(F)c(C(=O)Oc2ccc(Cl)c(Cl)c2)c1F

Mol. weight [g/mol]: 317.12

Physical Properties

Property code	Value	Unit	Source
gf	-403.73	kJ/mol	Joback Method
hf	-585.08	kJ/mol	Joback Method
hfus	35.49	kJ/mol	Joback Method
hvap	70.91	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	4.799		Crippen Method
mcvol	196.060	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
rinpol	2167.00		NIST Webbook
tb	747.67	K	Joback Method
tc	978.33	K	Joback Method
tf	496.16	K	Joback Method
vc	0.761	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.31	J/mol×K	747.67	Joback Method
cpg	483.11	J/mol×K	786.11	Joback Method
cpg	493.02	J/mol×K	824.56	Joback Method
cpg	502.07	J/mol×K	863.00	Joback Method
cpg	510.27	J/mol×K	901.45	Joback Method
cpg	517.65	J/mol×K	939.89	Joback Method
cpg	524.21	J/mol×K	978.33	Joback Method

Sources

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=U357686&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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