2,6-Difluoro-3-methylbenzoic acid, 4-chloro-2-methylphenyl ester

Inchi: InChI=1S/C15H11ClF2O2/c1-8-3-5-11(17)13(14(8)18)15(19)20-12-6-4-10(16)7-9(12)2/h3

InchiKey: MOBJPHUSMMTUBV-UHFFFAOYSA-N

Formula: C15H11ClF2O2

SMILES: Cc1cc(Cl)ccc1OC(=O)c1c(F)ccc(C)c1F

Mol. weight [g/mol]: 296.70

Physical Properties

Property code	Value	Unit	Source
gf	-383.38	kJ/mol	Joback Method
hf	-589.98	kJ/mol	Joback Method
hfus	33.89	kJ/mol	Joback Method
hvap	68.75	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.454		Crippen Method
mcvol	197.910	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
rinpol	2066.00		NIST Webbook
tb	733.12	K	Joback Method
tc	957.24	K	Joback Method
tf	477.51	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.74	J/mol×K	733.12	Joback Method
cpg	514.14	J/mol×K	770.47	Joback Method
cpg	525.62	J/mol×K	807.83	Joback Method
cpg	536.21	J/mol×K	845.18	Joback Method
cpg	545.91	J/mol×K	882.54	Joback Method
cpg	554.75	J/mol×K	919.89	Joback Method
cpg	562.75	J/mol×K	957.24	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=U343757&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