2,6-Difluoro-3-methylbenzamide, N-(3-chloro-4-fluorophenyl)-

Inchi: InChI=1S/C14H9ClF3NO/c1-7-2-4-11(17)12(13(7)18)14(20)19-8-3-5-10(16)9(15)6-8/h2-6

InchiKey: PLFZIWCDIKVLHR-UHFFFAOYSA-N

Formula: C14H9ClF3NO

SMILES: Cc1ccc(F)c(C(=O)Nc2ccc(F)c(Cl)c2)c1F

Mol. weight [g/mol]: 299.68

Physical Properties

Property code	Value	Unit	Source
gf	-392.22	kJ/mol	Joback Method
hf	-579.76	kJ/mol	Joback Method
hfus	38.29	kJ/mol	Joback Method
hvap	69.74	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	4.318		Crippen Method
mcvol	189.700	ml/mol	McGowan Method
pc	2331.52	kPa	Joback Method
rinpol	2290.00		NIST Webbook
tb	737.26	K	Joback Method
tc	957.29	K	Joback Method
tf	497.26	K	Joback Method
vc	0.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.42	J/mol×K	737.26	Joback Method
cpg	493.52	J/mol×K	773.93	Joback Method
cpg	503.79	J/mol×K	810.60	Joback Method
cpg	513.26	J/mol×K	847.28	Joback Method
cpg	521.95	J/mol×K	883.95	Joback Method
cpg	529.90	J/mol×K	920.62	Joback Method
cpg	537.15	J/mol×K	957.29	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=U358104&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