4-Fluoro-2-trifluoromethylbenzamide, N-(3-chloro-4-fluorophenyl)-

Inchi: InChI=1S/C14H7ClF5NO/c15-11-6-8(2-4-12(11)17)21-13(22)9-3-1-7(16)5-10(9)14(18,19)

InchiKey: LPLTYCOMVJSMNK-UHFFFAOYSA-N

Formula: C14H7ClF5NO

SMILES: O=C(Nc1ccc(F)c(Cl)c1)c1ccc(F)cc1C(F)(F)F

Mol. weight [g/mol]: 335.66

Physical Properties

Property code	Value	Unit	Source
gf	-769.37	kJ/mol	Joback Method
hf	-969.26	kJ/mol	Joback Method
hfus	37.42	kJ/mol	Joback Method
hvap	66.14	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	4.889		Crippen Method
mcvol	193.240	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	2053.00		NIST Webbook
rinpol	2053.00		NIST Webbook
tb	727.59	K	Joback Method
tc	940.24	K	Joback Method
tf	488.34	K	Joback Method
vc	0.772	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.53	J/mol×K	727.59	Joback Method
cpg	512.93	J/mol×K	763.03	Joback Method
cpg	522.47	J/mol×K	798.47	Joback Method
cpg	531.23	J/mol×K	833.92	Joback Method
cpg	539.24	J/mol×K	869.36	Joback Method
cpg	546.58	J/mol×K	904.80	Joback Method
cpg	553.30	J/mol×K	940.24	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=U358092&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