2-Fluoro-6-trifluoromethylbenzamide, N-(4-fluorophenyl)-

Inchi: InChI=1S/C14H8F5NO/c15-8-4-6-9(7-5-8)20-13(21)12-10(14(17,18)19)2-1-3-11(12)16/h1

InchiKey: LLSVKGMYXHFRLQ-UHFFFAOYSA-N

Formula: C14H8F5NO

SMILES: O=C(Nc1ccc(F)cc1)c1c(F)cccc1C(F)(F)F

Mol. weight [g/mol]: 301.21

Physical Properties

Property code	Value	Unit	Source
gf	-747.81	kJ/mol	Joback Method
hf	-942.05	kJ/mol	Joback Method
hfus	33.61	kJ/mol	Joback Method
hvap	61.10	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.236		Crippen Method
mcvol	181.000	ml/mol	McGowan Method
pc	2322.54	kPa	Joback Method
rinpol	1885.00		NIST Webbook
tb	685.18	K	Joback Method
tc	893.70	K	Joback Method
tf	445.90	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.02	J/mol×K	685.18	Joback Method
cpg	492.67	J/mol×K	719.93	Joback Method
cpg	503.41	J/mol×K	754.69	Joback Method
cpg	513.29	J/mol×K	789.44	Joback Method
cpg	522.37	J/mol×K	824.20	Joback Method
cpg	530.70	J/mol×K	858.95	Joback Method
cpg	538.36	J/mol×K	893.70	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=U358113&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