2-Fluoro-3-(trifluoromethyl)benzamide

Inchi: InChI=1S/C8H5F4NO/c9-6-4(7(13)14)2-1-3-5(6)8(10,11)12/h1-3H,(H2,13,14)
InchiKey: UHMUBYIIPNQHGD-UHFFFAOYSA-N
Formula: C8H5F4NO
SMILES: NC(=O)c1cccc(C(F)(F)F)c1F
Mol. weight [g/mol]: 207.12
CAS: 207853-60-9

Physical Properties

Property code	Value	Unit	Source
gf	-729.24	kJ/mol	Joback Method
hf	-866.84	kJ/mol	Joback Method
hfus	21.44	kJ/mol	Joback Method
hvap	49.83	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	1.943		Crippen Method
mcvol	118.450	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
tb	539.33	K	Joback Method
tc	743.04	K	Joback Method
tf	369.35	K	Joback Method
vc	0.471	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.33	J/mol×K	539.33	Joback Method
cpg	288.93	J/mol×K	573.28	Joback Method
cpg	297.83	J/mol×K	607.23	Joback Method
cpg	306.08	J/mol×K	641.18	Joback Method
cpg	313.70	J/mol×K	675.14	Joback Method
cpg	320.73	J/mol×K	709.09	Joback Method
cpg	327.21	J/mol×K	743.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C207853609&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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