3-Fluoro-5-(trifluoromethyl)benzylamine

Inchi: InChI=1S/C8H7F4N/c9-7-2-5(4-13)1-6(3-7)8(10,11)12/h1-3H,4,13H2
InchiKey: ADHUUMWSWNPEMZ-UHFFFAOYSA-N
Formula: C8H7F4N
SMILES: NCc1cc(F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 193.14
CAS: 150517-77-4

Physical Properties

Property code	Value	Unit	Source
gf	-600.32	kJ/mol	Joback Method
hf	-754.26	kJ/mol	Joback Method
hfus	19.84	kJ/mol	Joback Method
hvap	43.08	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.303		Crippen Method
mcvol	116.880	ml/mol	McGowan Method
pc	3124.49	kPa	Joback Method
tb	485.46	K	Joback Method
tc	679.96	K	Joback Method
tf	319.42	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.44	J/mol×K	485.46	Joback Method
cpg	276.27	J/mol×K	517.88	Joback Method
cpg	286.40	J/mol×K	550.29	Joback Method
cpg	295.87	J/mol×K	582.71	Joback Method
cpg	304.70	J/mol×K	615.12	Joback Method
cpg	312.94	J/mol×K	647.54	Joback Method
cpg	320.60	J/mol×K	679.96	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=C150517774&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume