3,5-(CF3)2C6H3N(CH3)2

Inchi: InChI=1S/C10H9F6N/c1-17(2)8-4-6(9(11,12)13)3-7(5-8)10(14,15)16/h3-5H,1-2H3
InchiKey: UHEAXRJEZXIZAT-UHFFFAOYSA-N
Formula: C10H9F6N
SMILES: CN(C)c1cc(C(F)(F)F)cc(C(F)(F)F)c1
Mol. weight [g/mol]: 257.18
CAS: 34060-81-6

Physical Properties

Property code	Value	Unit	Source
affp	884.90	kJ/mol	NIST Webbook
basg	858.40	kJ/mol	NIST Webbook
gf	-925.93	kJ/mol	Joback Method
hf	-1162.77	kJ/mol	Joback Method
hfus	21.59	kJ/mol	Joback Method
hvap	36.00	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.790		Crippen Method
mcvol	148.600	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
tb	466.44	K	Joback Method
tc	636.55	K	Joback Method
tf	294.77	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	344.99	J/mol×K	466.44	Joback Method
cpg	358.45	J/mol×K	494.79	Joback Method
cpg	371.06	J/mol×K	523.14	Joback Method
cpg	382.86	J/mol×K	551.49	Joback Method
cpg	393.89	J/mol×K	579.85	Joback Method
cpg	404.19	J/mol×K	608.20	Joback Method
cpg	413.81	J/mol×K	636.55	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=C34060816&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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