4-CF3C6H4N(CH3)2

Inchi: InChI=1S/C9H10F3N/c1-13(2)8-5-3-7(4-6-8)9(10,11)12/h3-6H,1-2H3
InchiKey: MLFFPCMQWLVVLM-UHFFFAOYSA-N
Formula: C9H10F3N
SMILES: CN(C)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 189.18
CAS: 329-17-9

Physical Properties

Property code	Value	Unit	Source
affp	903.20	kJ/mol	NIST Webbook
basg	876.80	kJ/mol	NIST Webbook
gf	-343.13	kJ/mol	Joback Method
hf	-533.58	kJ/mol	Joback Method
hfus	17.57	kJ/mol	Joback Method
hvap	36.86	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.771		Crippen Method
mcvol	129.200	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
tb	444.00	K	Joback Method
tc	630.76	K	Joback Method
tf	266.79	K	Joback Method
vc	0.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.63	J/mol×K	444.00	Joback Method
cpg	287.47	J/mol×K	475.13	Joback Method
cpg	300.46	J/mol×K	506.25	Joback Method
cpg	312.61	J/mol×K	537.38	Joback Method
cpg	323.99	J/mol×K	568.51	Joback Method
cpg	334.61	J/mol×K	599.64	Joback Method
cpg	344.54	J/mol×K	630.76	Joback Method

Sources

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=C329179&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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