Benzenamine, 2,3,4,5,6-pentafluoro-N,N-dimethyl-

Inchi: InChI=1S/C8H6F5N/c1-14(2)8-6(12)4(10)3(9)5(11)7(8)13/h1-2H3
InchiKey: KGTLSNJIWZULPZ-UHFFFAOYSA-N
Formula: C8H6F5N
SMILES: CN(C)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 211.13
CAS: 1801-14-5

Physical Properties

Property code	Value	Unit	Source
gf	-782.53	kJ/mol	Joback Method
hf	-942.29	kJ/mol	Joback Method
hfus	26.99	kJ/mol	Joback Method
hvap	36.95	kJ/mol	Joback Method
ie	8.48	eV	NIST Webbook
log10ws	-3.04		Crippen Method
logp	2.448		Crippen Method
mcvol	118.650	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
tb	442.81	K	Joback Method
tc	607.31	K	Joback Method
tf	304.36	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.68	J/mol×K	442.81	Joback Method
cpg	259.62	J/mol×K	470.23	Joback Method
cpg	268.22	J/mol×K	497.64	Joback Method
cpg	276.47	J/mol×K	525.06	Joback Method
cpg	284.39	J/mol×K	552.48	Joback Method
cpg	291.98	J/mol×K	579.89	Joback Method
cpg	299.25	J/mol×K	607.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1801145&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
ie:	Ionization energy
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