Dimethyl(2,2-difluoroethyl)amine

Inchi: InChI=1S/C4H8F3N/c1-8(2)3-4(5,6)7/h3H2,1-2H3
InchiKey: PVSHBYHMVOHXIM-UHFFFAOYSA-N
Formula: C4H8F3N
SMILES: CN(C)CC(F)(F)F
Mol. weight [g/mol]: 127.11
CAS: 819-06-7

Physical Properties

Property code	Value	Unit	Source
affp	902.70	kJ/mol	NIST Webbook
basg	871.90	kJ/mol	NIST Webbook
gf	-488.01	kJ/mol	Joback Method
hf	-655.44	kJ/mol	Joback Method
hfus	10.96	kJ/mol	Joback Method
hvap	22.79	kJ/mol	Joback Method
ie	8.42 ± 0.03	eV	NIST Webbook
ie	8.20	eV	NIST Webbook
log10ws	-0.73		Crippen Method
logp	1.110		Crippen Method
mcvol	82.510	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
tb	297.94	K	Joback Method
tc	442.35	K	Joback Method
tf	171.50	K	Joback Method
vc	0.321	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	139.15	J/mol×K	297.94	Joback Method
cpg	148.50	J/mol×K	322.01	Joback Method
cpg	157.43	J/mol×K	346.08	Joback Method
cpg	165.95	J/mol×K	370.14	Joback Method
cpg	174.06	J/mol×K	394.21	Joback Method

cpg	181.78	J/mol×K	418.28	Joback Method
cpg	189.13	J/mol×K	442.35	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=C819067&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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