Benzonitrile, 2,6-difluoro-

Other names: 2,6-Difluorobenzonitrile
Inchi: InChI=1S/C7H3F2N/c8-6-2-1-3-7(9)5(6)4-10/h1-3H
InchiKey: BNBRIFIJRKJGEI-UHFFFAOYSA-N
Formula: C7H3F2N
SMILES: N#Cc1c(F)cccc1F
Mol. weight [g/mol]: 139.10
CAS: 1897-52-5

Physical Properties

Property code	Value	Unit	Source
gf	-155.23	kJ/mol	Joback Method
hf	-201.56	kJ/mol	Joback Method
hfus	14.81	kJ/mol	Joback Method
hvap	43.62	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.836		Crippen Method
mcvol	90.650	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
tb	496.82	K	Joback Method
tc	710.74	K	Joback Method
tf	286.28	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.98	J/mol×K	496.82	Joback Method
cpg	184.39	J/mol×K	532.47	Joback Method
cpg	191.36	J/mol×K	568.13	Joback Method
cpg	197.91	J/mol×K	603.78	Joback Method
cpg	204.05	J/mol×K	639.43	Joback Method
cpg	209.79	J/mol×K	675.08	Joback Method
cpg	215.16	J/mol×K	710.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1897525&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

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