3,5-Difluorophenylacetonitrile

Inchi: InChI=1S/C8H5F2N/c9-7-3-6(1-2-11)4-8(10)5-7/h3-5H,1H2
InchiKey: OBMYMTSBABEPIB-UHFFFAOYSA-N
Formula: C8H5F2N
SMILES: N#CCc1cc(F)cc(F)c1
Mol. weight [g/mol]: 153.13
CAS: 122376-76-5

Physical Properties

Property code	Value	Unit	Source
gf	-146.81	kJ/mol	Joback Method
hf	-222.20	kJ/mol	Joback Method
hfus	17.40	kJ/mol	Joback Method
hvap	45.85	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.031		Crippen Method
mcvol	104.740	ml/mol	McGowan Method
pc	3086.42	kPa	Joback Method
tb	519.70	K	Joback Method
tc	730.29	K	Joback Method
tf	297.55	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.22	J/mol×K	519.70	Joback Method
cpg	225.89	J/mol×K	554.80	Joback Method
cpg	234.05	J/mol×K	589.90	Joback Method
cpg	241.73	J/mol×K	624.99	Joback Method
cpg	248.94	J/mol×K	660.09	Joback Method
cpg	255.71	J/mol×K	695.19	Joback Method
cpg	262.04	J/mol×K	730.29	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=C122376765&Units=SI

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