3,5-Difluoroacetonitrile

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

Physical Properties

Property code	Value	Unit	Source
hfus	17.40	kJ/mol	Joback Method
hvap	61.68	kJ/mol	Cheméo Relay (1.0)
ie	9.76	eV	Cheméo Relay (1.0)
logp	2.031		Crippen Method
mcvol	104.740	ml/mol	McGowan Method
tb	471.05	K	Cheméo Relay (1.0)
tf	288.54	K	Cheméo Relay (1.0)

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C122376765&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point