3-(Trifluoromethoxy)benzonitrile

Inchi: InChI=1S/C8H4F3NO/c9-8(10,11)13-7-3-1-2-6(4-7)5-12/h1-4H
InchiKey: DCZAPXGEZYVQNX-UHFFFAOYSA-N
Formula: C8H4F3NO
SMILES: N#Cc1cccc(OC(F)(F)F)c1
Mol. weight [g/mol]: 187.12
CAS: 52771-22-9

Physical Properties

Property code	Value	Unit	Source
gf	-434.15	kJ/mol	Joback Method
hf	-547.81	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	45.48	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	2.457		Crippen Method
mcvol	112.380	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
tb	533.18	K	Joback Method
tc	742.83	K	Joback Method
tf	310.27	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.03	J/mol×K	533.18	Joback Method
cpg	260.11	J/mol×K	568.12	Joback Method
cpg	268.54	J/mol×K	603.06	Joback Method
cpg	276.35	J/mol×K	638.00	Joback Method
cpg	283.59	J/mol×K	672.95	Joback Method
cpg	290.26	J/mol×K	707.89	Joback Method
cpg	296.41	J/mol×K	742.83	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=C52771229&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