

4-Chloro-3-cyanobenzotrifluoride

Other names:	Benzonitrile, 2-chloro-5-(trifluoromethyl)- 2-Chloro-5-(trifluoromethyl)benzonitrile
Inchi:	InChI=1S/C8H3ClF3N/c9-7-2-1-6(8(10,11)12)3-5(7)4-13/h1-3H
InchiKey:	LCISFYAQKHOWBP-UHFFFAOYSA-N
Formula:	C8H3ClF3N
SMILES:	N#Cc1cc(C(F)(F)F)ccc1Cl
Mol. weight [g/mol]:	205.56
CAS:	328-87-0

Physical Properties

Property code	Value	Unit	Source
gf	-350.71	kJ/mol	Joback Method
hf	-442.80	kJ/mol	Joback Method
hfus	17.27	kJ/mol	Joback Method
hvap	48.12	kJ/mol	Joback Method
log10ws	-3.61		Crippen Method
logp	3.230		Crippen Method
mvol	118.750	ml/mol	McGowan Method
pc	2881.21	kPa	Joback Method
tb	553.17	K	Joback Method
tc	770.81	K	Joback Method
tf	330.48	K	Joback Method
vc	0.493	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.69	J/mol×K	553.17	Joback Method
cpg	258.81	J/mol×K	589.44	Joback Method
cpg	266.27	J/mol×K	625.72	Joback Method
cpg	273.10	J/mol×K	661.99	Joback Method
cpg	279.36	J/mol×K	698.27	Joback Method
cpg	285.09	J/mol×K	734.54	Joback Method
cpg	290.33	J/mol×K	770.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C328870&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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

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