

Benzonitrile, 2-chloro-6-methyl-

Other names:	o-Tolunitrile, 6-chloro- 2-Chloro-6-methylbenzonitrile 2-Cyano-3-chlorotoluene 3-Chloro-2-tolunitrile
Inchi:	InChI=1S/C8H6ClN/c1-6-3-2-4-8(9)7(6)5-10/h2-4H,1H3
InchiKey:	WQWQHJNUHQEGTN-UHFFFAOYSA-N
Formula:	C8H6ClN
SMILES:	Cc1cccc(Cl)c1C#N
Mol. weight [g/mol]:	151.59
CAS:	6575-09-3

Physical Properties

Property code	Value	Unit	Source
gf	230.88	kJ/mol	Joback Method
hf	154.28	kJ/mol	Joback Method
hfus	15.44	kJ/mol	Joback Method
hvap	51.86	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.520		Crippen Method
mcvol	113.440	ml/mol	McGowan Method
pc	3276.53	kPa	Joback Method
tb	558.59	K	Joback Method
tc	797.23	K	Joback Method
tf	326.29	K	Joback Method
vc	0.451	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.61	J/molxK	558.59	Joback Method
cpg	230.58	J/molxK	598.36	Joback Method
cpg	238.96	J/molxK	638.14	Joback Method
cpg	246.78	J/molxK	677.91	Joback Method
cpg	254.06	J/molxK	717.68	Joback Method

cpg	260.81	J/mol×K	757.46	Joback Method
cpg	267.08	J/mol×K	797.23	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	416.20	K	5.10	NIST Webbook

Sources

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=C6575093&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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