Benzeneacetonitrile, 2,3,6-trichloro-

Other names:	Acetonitrile, (2,3,6-trichlorophenyl)-
	2,3,6-Trichlorobenzyl cyanide
	2,3,6-Trichlorophenylacetonitrile
Inchi:	InChI=1S/C8H4Cl3N/c9-6-1-2-7(10)8(11)5(6)3-4-12/h1-2H,3H2
InchiKey:	ZUZLGSONCFESPE-UHFFFAOYSA-N
Formula:	C8H4Cl3N
SMILES:	N#CCc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	220.48
CAS:	3215-65-4

Physical Properties

Property code	Value	Unit	Source
gf	197.39	kJ/mol	Joback Method
hf	111.33	kJ/mol	Joback Method
hfus	23.45	kJ/mol	Joback Method
hvap	61.30	kJ/mol	Joback Method
log10ws	-4.20		Crippen Method
logp	3.713		Crippen Method
mcvol	137.920	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
tb	638.43	K	Joback Method
tc	885.00	K	Joback Method
tf	398.65	K	Joback Method
vc	0.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.69	J/mol×K	638.43	Joback Method
cpg	265.91	J/mol×K	679.53	Joback Method
cpg	272.61	J/mol×K	720.62	Joback Method
cpg	278.79	J/mol×K	761.72	Joback Method
cpg	284.48	J/mol×K	802.81	Joback Method
cpg	289.70	J/mol×K	843.91	Joback Method

cpg	294.48	J/mol×K	885.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3215654&Units=SI
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

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