Benzenepropanenitrile, «alpha»,3-dichloro-2-methyl-

Other names:	CCTP
	FMC 28979
	Hydrocinnamonitrile, «alpha»,3-Dichloro-2-methyl-
	Orthonil
	PRB 8
	PRB 200
	2-Chloro-3-(3-chloro-o-tolyl)-propionitrile
	Bi-Act
	Propionitrile, 2-chloro-3-(3-chloro-o-tolyl)-
	NSC 239071
	2-(2-Chloro-2-cyanoethyl)-6-chlorotolyl
	2-chloro-3-(m-chloro-o-tolyl)propionitrile
Inchi:	InChI=1S/C10H9Cl2N/c1-7-8(5-9(11)6-13)3-2-4-10(7)12/h2-4,9H,5H2,1H3
InchiKey:	YYJUXSGXHHPBTK-UHFFFAOYSA-N
Formula:	C10H9Cl2N
SMILES:	Cc1c(Cl)cccc1CC(Cl)C#N
Mol. weight [g/mol]:	214.09
CAS:	21342-85-8

Physical Properties

Property code	Value	Unit	Source
gf	233.35	kJ/mol	Joback Method
hf	91.98	kJ/mol	Joback Method
hfus	21.30	kJ/mol	Joback Method
hvap	60.31	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.322		Crippen Method
mcvol	153.860	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
tb	641.34	K	Joback Method
tc	878.81	K	Joback Method
tf	363.75	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.07	J/mol×K	641.34	Joback Method
cpg	343.57	J/mol×K	680.92	Joback Method
cpg	353.34	J/mol×K	720.50	Joback Method
cpg	362.39	J/mol×K	760.08	Joback Method
cpg	370.78	J/mol×K	799.65	Joback Method
cpg	378.53	J/mol×K	839.23	Joback Method
cpg	385.67	J/mol×K	878.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	384.20	K	0.07	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C21342858&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume