2-Chlorobenzalmalononitrile

Other names:	CS Propanedinitrile, [(2-chlorophenyl)methylene]- Malononitrile, (o-chlorobenzylidene)- «beta»,«beta»-Dicyano-o-chlorostyrene (o-Chlorobenzal)malononitrile (o-Chlorobenzylidene)malononitrile 2-Chlorobenzylidenemalononitrile (o-Chlorobenzylidene)malonitrile o-Chlorobenzylidenemalonic nitrile NCI-C55118 USAF KF-11 2-Chloro BMN beta,bbeta-Dicyano-o-chlorostyrene 2-Chlorobenzylidenemaloninitrile CS (lacrimator) NSC 542 Propanedinitrile, 2-[(2-chlorophenyl)methylene]- 2-Chlorobenzylmalonodinitrile [(2-chlorophenyl)methylene]malononitrile
Inchi:	InChI=1S/C10H5ClN2/c11-10-4-2-1-3-9(10)5-8(6-12)7-13/h1-5H
InchiKey:	JJNZXLAFIPKXIG-UHFFFAOYSA-N
Formula:	C10H5ClN2
SMILES:	N#CC(C#N)=Cc1ccccc1Cl
Mol. weight [g/mol]:	188.61
CAS:	2698-41-1

Physical Properties

Property code	Value	Unit	Source
gf	462.20	kJ/mol	Joback Method
hf	396.78	kJ/mol	Joback Method
hfus	21.41	kJ/mol	Joback Method
hvap	66.17	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	2.771		Crippen Method
mcvol	138.700	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
rinpol	1562.09		NIST Webbook

rinpol	1516.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1561.60		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1562.09		NIST Webbook
rinpol	1554.28		NIST Webbook
rinpol	1554.40		NIST Webbook
rinpol	1555.10		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1554.40		NIST Webbook
tb	705.49	K	Joback Method
tc	960.44	K	Joback Method
tf	382.26	K	Joback Method
vc	0.570	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.16	J/mol×K	705.49	Joback Method
cpg	308.11	J/mol×K	747.98	Joback Method
cpg	315.40	J/mol×K	790.47	Joback Method
cpg	322.09	J/mol×K	832.96	Joback Method
cpg	328.27	J/mol×K	875.45	Joback Method
cpg	334.00	J/mol×K	917.94	Joback Method
cpg	339.35	J/mol×K	960.44	Joback Method

Sources

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=C2698411&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume