A-CHLOROBENZALMALONODINITRILE

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]:	188.62

Physical Properties

Property code	Value	Unit	Source
hfus	21.41	kJ/mol	Joback Method
ie	9.45	eV	Cheméo Relay (1.0)
logp	2.771		Crippen Method
mcvol	138.700	ml/mol	McGowan Method
rinpol	1561.60		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1562.09		NIST Webbook

rinpol	1562.09		NIST Webbook
rinpol	1554.28		NIST Webbook
rinpol	1554.40		NIST Webbook
rinpol	1555.10		NIST Webbook
rinpol	1554.40		NIST Webbook
rinpol	1516.00		NIST Webbook
rinpol	1564.00		NIST Webbook
tb	542.62	K	Cheméo Relay (1.0)
tf	333.78	K	Cheméo Relay (1.0)

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2698411&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
hfus: Enthalpy of fusion at standard conditions

ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point