

Benzene, 1-chloro-4-(2,2-dicyanoethenyl)

Other names:	p-Chlorobenzylidenemalononitrile Malononitrile, (p-chlorobenzylidene)- Propanedinitrile, ((4-chlorophenyl)methylene)- 4-Chlorobenzalmalononitrile 4-Chlorobenzylidenemalononitrile 4-Chlor-benzal-malonitril F 2371 2-(4-Chlorobenzylidene)malononitrile Malonodinitrile, 4-chlorobenzylidene NSC 492
Inchi:	InChI=1S/C10H5ClN2/c11-10-3-1-8(2-4-10)5-9(6-12)7-13/h1-5H
InchiKey:	FQSXBLOWLYPURG-UHFFFAOYSA-N
Formula:	C10H5ClN2
SMILES:	N#CC(C#N)=Cc1ccc(Cl)cc1
Mol. weight [g/mol]:	188.61
CAS:	1867-38-5

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	1565.00		NIST Webbook
tb	705.49	K	Joback Method
tc	960.44	K	Joback Method
tf	382.26	K	Joback Method
vc	0.570	m ³ /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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C1867385&Units=SI

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

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