

BENZENE, 1-CHLORO-4-(2,2-DICYANOETHENYL)

Other names: 2-(4-Chlorobenzylidene)malononitrile
4-Chlor-benzal-malonitril
4-Chlorobenzal-malononitrile
4-Chlorobenzylidenemalononitrile
F 2371
Malonodinitrile, 4-chlorobenzylidene
Malononitrile, (p-chlorobenzylidene)-
NSC 492
Propanedinitrile, ((4-chlorophenyl)methylene)-
p-Chlorobenzylidenemalononitrile

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]: 188.62

Physical Properties

Property code	Value	Unit	Source
hfus	21.41	kJ/mol	Joback Method
ie	9.36	eV	Cheméo Relay (1.0)
logp	2.771		Crippen Method
mcvol	138.700	ml/mol	McGowan Method
tb	554.09	K	Cheméo Relay (1.0)
tf	380.37	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

Sources

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=C1867385&Units=SI
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
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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