

Pentanedinitrile, 2-methylene-

Other names:	Methylene glutaronitrile 2-Methyleneglutaronitrile 2,4-Dicyanobutene-1 Glutaronitrile, 2-methylene- «alpha»-Methyleneglutaronitrile 2,4-Dicyano-1-butene «alpha»-Methyleneglutarodinitrile 2-Methyleneglutarodinitrile 2-Methylenepentanedinitrile
Inchi:	InChI=1S/C6H6N2/c1-6(5-8)3-2-4-7/h1-3H2
InchiKey:	NGCJVMZXRCLPRQ-UHFFFAOYSA-N
Formula:	C6H6N2
SMILES:	C=C(C#N)CCC#N
Mol. weight [g/mol]:	106.13
CAS:	1572-52-7

Physical Properties

Property code	Value	Unit	Source
gf	345.29	kJ/mol	Joback Method
hf	278.23	kJ/mol	Joback Method
hfus	11.72	kJ/mol	Joback Method
hvap	49.32	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	1.370		Crippen Method
mcvol	93.860	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	1023.00		NIST Webbook
rinpol	1023.00		NIST Webbook
tb	376.20	K	NIST Webbook
tc	753.93	K	Joback Method
tf	271.64	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.84	J/mol×K	537.40	Joback Method
cpg	196.69	J/mol×K	573.49	Joback Method
cpg	203.15	J/mol×K	609.58	Joback Method
cpg	209.23	J/mol×K	645.66	Joback Method
cpg	214.96	J/mol×K	681.75	Joback Method
cpg	220.36	J/mol×K	717.84	Joback Method
cpg	225.43	J/mol×K	753.93	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=C1572527&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

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