3-Methylenecyclobutanenitrile

Other names: Cyclobutanecarbonitrile,3-methylene-,
3-Methylenecyclobutane-carbonitrile
Inchi: InChI=1S/C6H7N/c1-5-2-6(3-5)4-7/h6H,1-3H2
InchiKey: ZRWMAMOBIQQJSA-UHFFFAOYSA-N
Formula: C6H7N
SMILES: C=C1CC(C#N)C1
Mol. weight [g/mol]: 93.13
CAS: 15760-35-7

Physical Properties

Property code	Value	Unit	Source
chl	-3569.40 ± 2.10	kJ/mol	NIST Webbook
gf	234.55	kJ/mol	Joback Method
hf	252.40	kJ/mol	NIST Webbook
hfl	207.90	kJ/mol	NIST Webbook
hfus	7.68	kJ/mol	Joback Method
hvap	44.56	kJ/mol	NIST Webbook
hvap	44.50	kJ/mol	NIST Webbook
log10ws	-1.71		Crippen Method
logp	1.476		Crippen Method
mcvol	81.620	ml/mol	McGowan Method
pc	3695.46	kPa	Joback Method
tb	448.93	K	Joback Method
tc	663.99	K	Joback Method
tf	250.47	K	Joback Method
vc	0.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	157.75	J/mol×K	448.93	Joback Method
cpg	167.23	J/mol×K	484.77	Joback Method
cpg	176.15	J/mol×K	520.62	Joback Method
cpg	184.55	J/mol×K	556.46	Joback Method

cpg	192.44	J/mol×K	592.31	Joback Method
cpg	199.85	J/mol×K	628.15	Joback Method
cpg	206.81	J/mol×K	663.99	Joback Method
cpl	190.90	J/mol×K	297.00	NIST Webbook
hvapt	45.90	kJ/mol	391.50	NIST Webbook

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=C15760357&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume