

Cyclobutanecarbonitrile

Other names:	Cyanocyclobutane Cyclobutyl cyanide
Inchi:	InChI=1S/C5H7N/c6-4-5-2-1-3-5/h5H,1-3H2
InchiKey:	GFBLFDSCAKHHGX-UHFFFAOYSA-N
Formula:	C5H7N
SMILES:	N#CC1CCC1
Mol. weight [g/mol]:	81.12
CAS:	4426-11-3

Physical Properties

Property code	Value	Unit	Source
chl	-3071.00 ± 1.10	kJ/mol	NIST Webbook
gf	173.05	kJ/mol	Joback Method
hf	147.30 ± 1.10	kJ/mol	NIST Webbook
hf	143.00	kJ/mol	NIST Webbook
hfl	103.00	kJ/mol	NIST Webbook
hfus	6.25	kJ/mol	Joback Method
hvap	40.00	kJ/mol	NIST Webbook
hvap	40.00	kJ/mol	NIST Webbook
hvap	44.37	kJ/mol	NIST Webbook
hvap	44.34 ± 0.20	kJ/mol	NIST Webbook
hvap	44.30	kJ/mol	NIST Webbook
hvap	40.00 ± 0.40	kJ/mol	NIST Webbook
log10ws	-1.44		Crippen Method
logp	1.310		Crippen Method
mcvol	71.830	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
tb	422.70	K	NIST Webbook
tc	642.75	K	Joback Method
tf	225.52	K	Joback Method
vc	0.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	170.04	J/mol×K	570.80	Joback Method
cpg	177.61	J/mol×K	606.77	Joback Method
cpg	134.27	J/mol×K	426.89	Joback Method
cpg	144.10	J/mol×K	462.87	Joback Method
cpg	153.32	J/mol×K	498.84	Joback Method
cpg	161.95	J/mol×K	534.82	Joback Method
cpg	184.69	J/mol×K	642.75	Joback Method
cpl	146.00	J/mol×K	297.00	NIST Webbook
hvapt	36.88	kJ/mol	422.70	NIST Webbook
hvapt	39.60	kJ/mol	365.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C4426113&Units=SI

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

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