1,2-Cyclobutanedicarbonitrile, trans-

Other names:	trans-1,2-Cyclobutanedicarbonitrile
	trans-1,2-Dicyanocyclobutane
	USAF st-1
	1,2-Cyclobutanedicarbonitrile, (E)-
Inchi:	InChI=1S/C6H6N2/c7-3-5-1-2-6(5)4-8/h5-6H,1-2H2/t5-,6-/m1/s1
InchiKey:	CZPLUOCTUPJSIZ-PHDIDXHHSA-N
Formula:	C6H6N2
SMILES:	N#CC1CCC1C#N
Mol. weight [g/mol]:	106.13
CAS:	3211-20-9

Physical Properties

Property code	Value	Unit	Source
gf	306.94	kJ/mol	Joback Method
hf	208.89	kJ/mol	Joback Method
hfus	11.41	kJ/mol	Joback Method
hvap	49.68	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	1.060		Crippen Method
mcvol	87.300	ml/mol	McGowan Method
pc	3372.36	kPa	Joback Method
tb	547.18	K	Joback Method
tc	779.51	K	Joback Method
tf	297.54	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	194.51	J/mol×K	547.18	Joback Method
cpg	203.68	J/mol×K	585.90	Joback Method
cpg	212.25	J/mol×K	624.62	Joback Method
cpg	220.24	J/mol×K	663.35	Joback Method
cpg	227.68	J/mol×K	702.07	Joback Method

cpg	234.61	J/mol×K	740.79	Joback Method
cpg	241.05	J/mol×K	779.51	Joback Method

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=C3211209&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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