

1,3-Cyclobutanedicarbonitrile, 1,3-dihydroxy-2,2,4,4-tetramethyl-

Inchi:	InChI=1S/C10H14N2O2/c1-7(2)9(13,5-11)8(3,4)10(7,14)6-12/h13-14H,1-4H3
InchiKey:	FICLSLGHSTXBNR-UHFFFAOYSA-N
Formula:	C10H14N2O2
SMILES:	CC1(C)C(O)(C#N)C(C)(C)C1(O)C#N
Mol. weight [g/mol]:	194.23
CAS:	116373-47-8

Physical Properties

Property code	Value	Unit	Source
gf	29.60	kJ/mol	Joback Method
hf	-157.85	kJ/mol	Joback Method
hfus	6.90	kJ/mol	Joback Method
hvap	86.72	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	0.562		Crippen Method
mcvol	155.400	ml/mol	McGowan Method
pc	3059.17	kPa	Joback Method
tb	814.68	K	Joback Method
tc	1030.46	K	Joback Method
tf	551.38	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.62	J/molxK	814.68	Joback Method
cpg	477.40	J/molxK	850.64	Joback Method
cpg	492.83	J/molxK	886.61	Joback Method
cpg	510.27	J/molxK	922.57	Joback Method
cpg	530.09	J/molxK	958.54	Joback Method
cpg	552.64	J/molxK	994.50	Joback Method
cpg	578.28	J/molxK	1030.46	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=C116373478&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
mccvol:	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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