trans-1,4-Cyclohexanedicarbonitrile

Other names:	1,4-Cyclohexanedicarbonitrile, trans- trans-1,4-Dicyanocyclohexane 1,4-Cyclohexanedicarbonitrile, (E)- trans-1,4-Cyclohexane-carbonitrile
Inchi:	InChI=1S/C8H10N2/c9-5-7-1-2-8(6-10)4-3-7/h7-8H,1-4H2/t7-,8-
InchiKey:	MGWYSXZGBRHJNE-ZKCHVHJHSA-N
Formula:	C8H10N2
SMILES:	N#CC1CCC(C#N)CC1
Mol. weight [g/mol]:	134.18
CAS:	6550-85-2

Physical Properties

Property code	Value	Unit	Source
gf	299.58	kJ/mol	Joback Method
hf	155.29	kJ/mol	Joback Method
hfus	12.39	kJ/mol	Joback Method
hvap	54.48	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	1.840		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
pc	2878.12	kPa	Joback Method
tb	601.48	K	Joback Method
tc	841.10	K	Joback Method
tf	313.04	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.25	J/mol×K	601.48	Joback Method
cpg	297.20	J/mol×K	641.42	Joback Method
cpg	309.27	J/mol×K	681.35	Joback Method
cpg	320.49	J/mol×K	721.29	Joback Method
cpg	330.88	J/mol×K	761.23	Joback Method

cpg	340.45	J/mol×K	801.17	Joback Method
cpg	349.24	J/mol×K	841.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6550852&Units=SI
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

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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