

cis-1,2-Dimethylcycloheptane

Inchi:	InChI=1S/C9H18/c1-8-6-4-3-5-7-9(8)2/h8-9H,3-7H2,1-2H3/t8-,9+
InchiKey:	CLYDEJQPKBFLJW-DTORHVGOSA-N
Formula:	C9H18
SMILES:	CC1CCCCC1C
Mol. weight [g/mol]:	126.24
CAS:	13151-51-4

Physical Properties

Property code	Value	Unit	Source
gf	29.54	kJ/mol	Joback Method
hf	-201.27	kJ/mol	Joback Method
hfus	9.87	kJ/mol	Joback Method
hvap	35.92	kJ/mol	Joback Method
ie	10.21 ± 0.05	eV	NIST Webbook
ie	10.12	eV	NIST Webbook
log10ws	-3.00		Crippen Method
logp	3.223		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
rinpola	961.00		NIST Webbook
tb	424.47	K	Joback Method
tc	631.20	K	Joback Method
tf	190.81	K	Joback Method
vc	0.464	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.42	J/mol×K	424.47	Joback Method
cpg	274.39	J/mol×K	458.92	Joback Method
cpg	293.45	J/mol×K	493.38	Joback Method
cpg	311.63	J/mol×K	527.83	Joback Method
cpg	328.92	J/mol×K	562.29	Joback Method
cpg	345.35	J/mol×K	596.74	Joback Method

cpg	360.93	J/mol×K	631.20	Joback Method
dvisc	0.0086504	Paxs	190.81	Joback Method
dvisc	0.0028552	Paxs	229.75	Joback Method
dvisc	0.0012995	Paxs	268.70	Joback Method
dvisc	0.0007219	Paxs	307.64	Joback Method
dvisc	0.0004576	Paxs	346.58	Joback Method
dvisc	0.0003181	Paxs	385.53	Joback Method
dvisc	0.0002364	Paxs	424.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13151514&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
dvisc:	Dynamic viscosity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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