

Cycloheptene, 1,2-dimethyl-

Inchi:	InChI=1S/C9H16/c1-8-6-4-3-5-7-9(8)2/h3-7H2,1-2H3
InchiKey:	RNUMLXR VXVCOAQ-UHFFFAOYSA-N
Formula:	C9H16
SMILES:	CC1=C(C)CCCCC1
Mol. weight [g/mol]:	124.22
CAS:	20053-89-8

Physical Properties

Property code	Value	Unit	Source
gf	55.66	kJ/mol	Joback Method
hf	-125.75	kJ/mol	Joback Method
hfus	8.17	kJ/mol	Joback Method
hvap	38.15	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.287		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
tb	432.00 ± 6.00	K	NIST Webbook
tc	655.56	K	Joback Method
tf	225.09	K	Joback Method
vc	0.452	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.70	J/mol×K	442.93	Joback Method
cpg	260.82	J/mol×K	478.37	Joback Method
cpg	277.12	J/mol×K	513.81	Joback Method
cpg	292.62	J/mol×K	549.24	Joback Method
cpg	307.33	J/mol×K	584.68	Joback Method
cpg	321.28	J/mol×K	620.12	Joback Method
cpg	334.46	J/mol×K	655.56	Joback Method
dvisc	0.0059744	Paxs	225.09	Joback Method
dvisc	0.0023029	Paxs	261.40	Joback Method

dvisc	0.0011200	Paxs	297.70	Joback Method
dvisc	0.0006372	Paxs	334.01	Joback Method
dvisc	0.0004049	Paxs	370.32	Joback Method
dvisc	0.0002790	Paxs	406.62	Joback Method
dvisc	0.0002043	Paxs	442.93	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C20053898&Units=SI

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
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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