

(Z,Z)-1,5-Cyclooctadiene, 1-methyl

Inchi:

InChI=1S/C9H14/c1-9-7-5-3-2-4-6-8-9/h2-3,8H,4-7H2,1H3/b3-2-,9-8-

InchiKey:

HOEFIGOFJSMARD-FUOWLQLWSA-N

Formula:

C9H14

SMILES:

CC1=CCCC=CCC1

Mol. weight [g/mol]:

122.21

Physical Properties

Property code	Value	Unit	Source
gf	83.15	kJ/mol	Joback Method
hf	-62.66	kJ/mol	Joback Method
hfus	7.68	kJ/mol	Joback Method
hvap	37.96	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.063		Crippen Method
mcvol	118.210	ml/mol	McGowan Method
pc	3314.37	kPa	Joback Method
rinpol	998.00		NIST Webbook
tb	441.38	K	Joback Method
tc	663.63	K	Joback Method
tf	209.81	K	Joback Method
vc	0.429	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.98	J/mol×K	441.38	Joback Method
cpg	244.37	J/mol×K	478.42	Joback Method
cpg	260.85	J/mol×K	515.46	Joback Method
cpg	276.43	J/mol×K	552.51	Joback Method
cpg	291.13	J/mol×K	589.55	Joback Method
cpg	304.96	J/mol×K	626.59	Joback Method
cpg	317.94	J/mol×K	663.63	Joback Method
dvisc	0.0131293	Pa×s	209.81	Joback Method
dvisc	0.0036904	Pa×s	248.41	Joback Method

dvisc	0.0014593	Pa×s	287.00	Joback Method
dvisc	0.0007190	Pa×s	325.60	Joback Method
dvisc	0.0004116	Pa×s	364.19	Joback Method
dvisc	0.0002622	Pa×s	402.78	Joback Method
dvisc	0.0001807	Pa×s	441.38	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R3033&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
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
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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