Methylenecyclooctane

Other names: Cyclooctane, methylene-
Inchi: InChI=1S/C9H16/c1-9-7-5-3-2-4-6-8-9/h1-8H2
InchiKey: GQRWNDZUODCEAJ-UHFFFAOYSA-N
Formula: C9H16
SMILES: C=C1CCCCCCC1
Mol. weight [g/mol]: 124.22
CAS: 3618-18-6

Physical Properties

Property code	Value	Unit	Source
gf	85.94	kJ/mol	Joback Method
hf	-82.51	kJ/mol	Joback Method
hfus	4.47	kJ/mol	Joback Method
hvap	36.87	kJ/mol	Joback Method
ie	8.79	eV	NIST Webbook
log10ws	-3.34		Crippen Method
logp	3.287		Crippen Method
mcvol	122.510	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
tb	428.00 ± 1.00	K	NIST Webbook
tc	655.42	K	Joback Method
tf	209.45	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	239.94	J/mol×K	437.24	Joback Method
cpg	325.04	J/mol×K	619.06	Joback Method
cpg	309.84	J/mol×K	582.69	Joback Method
cpg	293.74	J/mol×K	546.33	Joback Method
cpg	276.73	J/mol×K	509.97	Joback Method
cpg	258.80	J/mol×K	473.60	Joback Method
cpg	339.36	J/mol×K	655.42	Joback Method

dvisc	0.0002104	Pa×s	437.24	Joback Method
dvisc	0.0003114	Pa×s	399.27	Joback Method
dvisc	0.0005007	Pa×s	361.31	Joback Method
dvisc	0.0008999	Pa×s	323.35	Joback Method
dvisc	0.0018905	Pa×s	285.38	Joback Method
dvisc	0.0049874	Pa×s	247.41	Joback Method
dvisc	0.0187026	Pa×s	209.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3618186&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume