Cyclooctane, methyl-

Other names: Methylcyclooctane
Inchi: InChI=1S/C9H18/c1-9-7-5-3-2-4-6-8-9/h9H,2-8H2,1H3
InchiKey: POCNHGFJLGYFIK-UHFFFAOYSA-N
Formula: C9H18
SMILES: CC1CCCCCCC1
Mol. weight [g/mol]: 126.24
CAS: 1502-38-1

Physical Properties

Property code	Value	Unit	Source
gf	25.15	kJ/mol	Joback Method
hf	-187.09	kJ/mol	Joback Method
hfus	6.70	kJ/mol	Joback Method
hvap	36.40	kJ/mol	Joback Method
ie	9.70 ± 0.05	eV	NIST Webbook
log10ws	-3.24		Crippen Method
logp	3.367		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
rinpol	1009.00		NIST Webbook
rinpol	1019.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	995.00		NIST Webbook
tb	433.41	K	Joback Method
tc	649.15	K	Joback Method
tf	288.00 ± 5.00	K	NIST Webbook
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.12	J/mol×K	433.41	Joback Method

cpg	274.97	J/mol×K	469.37	Joback Method
cpg	294.81	J/mol×K	505.32	Joback Method
cpg	313.65	J/mol×K	541.28	Joback Method
cpg	331.52	J/mol×K	577.24	Joback Method
cpg	348.41	J/mol×K	613.19	Joback Method
cpg	364.35	J/mol×K	649.15	Joback Method
dvisc	0.0303341	Pa×s	191.53	Joback Method
dvisc	0.0064292	Pa×s	231.84	Joback Method
dvisc	0.0021577	Pa×s	272.16	Joback Method
dvisc	0.0009598	Pa×s	312.47	Joback Method
dvisc	0.0005138	Pa×s	352.78	Joback Method
dvisc	0.0003126	Pa×s	393.10	Joback Method
dvisc	0.0002086	Pa×s	433.41	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1502381&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
KDB: https://www.cheric.org/files/research/kdb/mol/mol581.mol

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