Methylenecycloheptane

Inchi: InChI=1S/C8H14/c1-8-6-4-2-3-5-7-8/h1-7H2
InchiKey: XJYOAWSHIQNEGC-UHFFFAOYSA-N
Formula: C8H14
SMILES: C=C1CCCCCC1
Mol. weight [g/mol]: 110.20
CAS: 2505-03-5

Physical Properties

Property code	Value	Unit	Source
gf	89.62	kJ/mol	Joback Method
hf	-55.71	kJ/mol	Joback Method
hfus	3.98	kJ/mol	Joback Method
hvap	34.47	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.897		Crippen Method
mcvol	108.420	ml/mol	McGowan Method
pc	3443.98	kPa	Joback Method
tb	412.00 ± 3.00	K	NIST Webbook
tb	408.00 ± 2.00	K	NIST Webbook
tb	406.00 ± 1.00	K	NIST Webbook
tc	622.03	K	Joback Method
tf	201.70	K	Joback Method
vc	0.394	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.83	J/mol×K	410.09	Joback Method
cpg	273.88	J/mol×K	586.71	Joback Method
cpg	260.42	J/mol×K	551.38	Joback Method
cpg	246.21	J/mol×K	516.06	Joback Method
cpg	231.22	J/mol×K	480.74	Joback Method
cpg	215.43	J/mol×K	445.41	Joback Method
cpg	286.58	J/mol×K	622.03	Joback Method

dvisc	0.0002573	Pa×s	410.09	Joback Method
dvisc	0.0003607	Pa×s	375.36	Joback Method
dvisc	0.0005416	Pa×s	340.63	Joback Method
dvisc	0.0008920	Pa×s	305.89	Joback Method
dvisc	0.0016692	Pa×s	271.16	Joback Method
dvisc	0.0037551	Pa×s	236.43	Joback Method
dvisc	0.0111689	Pa×s	201.70	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2505035&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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