

Cycloheptane, methylene

Inchi:	InChI=1S/C8H14/c1-8-6-4-2-3-5-7-8/h1-7H2
InchiKey:	XJYOAWSHIQNEGC-UHFFFAOYSA-N
Formula:	C8H14
SMILES:	C=C1CCCCC1
Mol. weight [g/mol]:	110.20

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
rinpola	861.00		NIST Webbook
tb	410.09	K	Joback Method
tc	622.03	K	Joback Method
tf	201.70	K	Joback Method
vc	0.394	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.83	J/molxK	410.09	Joback Method
cpg	215.43	J/molxK	445.41	Joback Method
cpg	231.22	J/molxK	480.74	Joback Method
cpg	246.21	J/molxK	516.06	Joback Method
cpg	260.42	J/molxK	551.38	Joback Method
cpg	273.88	J/molxK	586.71	Joback Method
cpg	286.58	J/molxK	622.03	Joback Method
dvisc	0.0111689	Paxs	201.70	Joback Method
dvisc	0.0037551	Paxs	236.43	Joback Method

dvisc	0.0016692	Paxs	271.16	Joback Method
dvisc	0.0008920	Paxs	305.89	Joback Method
dvisc	0.0005416	Paxs	340.63	Joback Method
dvisc	0.0003607	Paxs	375.36	Joback Method
dvisc	0.0002573	Paxs	410.09	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=R133116&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
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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