Cycloheptane, methyl-

Other names: Methylcycloheptane
Inchi: InChI=1S/C8H16/c1-8-6-4-2-3-5-7-8/h8H,2-7H2,1H3
InchiKey: GYNNXHKOJHMOHS-UHFFFAOYSA-N
Formula: C8H16
SMILES: CC1CCCCCC1
Mol. weight [g/mol]: 112.21
CAS: 4126-78-7

Physical Properties

Property code	Value	Unit	Source
gf	28.83	kJ/mol	Joback Method
hf	-160.29	kJ/mol	Joback Method
hfus	6.21	kJ/mol	Joback Method
hvap	34.00	kJ/mol	Joback Method
ie	9.70 ± 0.05	eV	NIST Webbook
log10ws	-2.82		Crippen Method
logp	2.977		Crippen Method
mcvol	112.720	ml/mol	McGowan Method
pc	3243.03	kPa	Joback Method
rinpol	908.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	864.00		NIST Webbook
rinpol	864.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	882.00		NIST Webbook
rinpol	860.00		NIST Webbook
rinpol	860.00		NIST Webbook
ripol	935.00		NIST Webbook
ripol	935.00		NIST Webbook
tb	407.00 ± 3.00	K	NIST Webbook
tb	407.00 ± 3.00	K	NIST Webbook
tb	407.00 ± 3.00	K	NIST Webbook
tb	407.20	K	NIST Webbook
tc	615.70	K	Joback Method
tf	183.78	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.56	J/mol×K	406.26	Joback Method
cpg	295.89	J/mol×K	580.80	Joback Method
cpg	280.72	J/mol×K	545.89	Joback Method
cpg	264.72	J/mol×K	510.98	Joback Method
cpg	247.87	J/mol×K	476.07	Joback Method
cpg	230.16	J/mol×K	441.17	Joback Method
cpg	310.24	J/mol×K	615.70	Joback Method
dvisc	0.0002515	Pa×s	406.26	Joback Method
dvisc	0.0003556	Pa×s	369.18	Joback Method
dvisc	0.0005433	Pa×s	332.10	Joback Method
dvisc	0.0009233	Pa×s	295.02	Joback Method
dvisc	0.0018277	Pa×s	257.94	Joback Method
dvisc	0.0045503	Pa×s	220.86	Joback Method
dvisc	0.0163689	Pa×s	183.78	Joback Method

Sources

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/mol479.mol
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4126787&Units=SI

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