1-Methylcycloheptene

Other names: Cycloheptene, 1-methyl-
Inchi: InChI=1S/C8H14/c1-8-6-4-2-3-5-7-8/h6H,2-5,7H2,1H3
InchiKey: MREBNFRVGNTYOV-UHFFFAOYSA-N
Formula: C8H14
SMILES: CC1=CCCCCC1
Mol. weight [g/mol]: 110.20
CAS: 1453-25-4

Physical Properties

Property code	Value	Unit	Source
gf	56.87	kJ/mol	Joback Method
hf	-93.64	kJ/mol	Joback Method
hfus	5.97	kJ/mol	Joback Method
hvap	35.27	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.897		Crippen Method
mcvol	108.420	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
rinpol	874.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	868.00		NIST Webbook
rinpol	863.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	874.00		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	909.00		NIST Webbook
tb	407.90 ± 4.00	K	NIST Webbook
tb	409.20 ± 2.00	K	NIST Webbook
tb	408.00 ± 3.00	K	NIST Webbook
tc	628.83	K	Joback Method
tf	201.30	K	Joback Method
vc	0.396	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	200.27	J/mol×K	415.07	Joback Method
cpg	274.56	J/mol×K	593.20	Joback Method
cpg	261.28	J/mol×K	557.58	Joback Method
cpg	247.23	J/mol×K	521.95	Joback Method
cpg	232.39	J/mol×K	486.32	Joback Method
cpg	216.74	J/mol×K	450.70	Joback Method
cpg	287.10	J/mol×K	628.83	Joback Method
dvisc	0.0002294	Pa×s	415.07	Joback Method
dvisc	0.0003223	Pa×s	379.44	Joback Method
dvisc	0.0004857	Pa×s	343.81	Joback Method
dvisc	0.0008048	Pa×s	308.18	Joback Method
dvisc	0.0015219	Pa×s	272.56	Joback Method
dvisc	0.0034856	Pa×s	236.93	Joback Method
dvisc	0.0107049	Pa×s	201.30	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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1453254&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
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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