Cycloheptane, 1,1-dimethyl

Inchi: InChI=1S/C9H18/c1-9(2)7-5-3-4-6-8-9/h3-8H2,1-2H3
InchiKey: CRGBHZNMDZJGAI-UHFFFAOYSA-N
Formula: C9H18
SMILES: CC1(C)CCCCCC1
Mol. weight [g/mol]: 126.24

Physical Properties

Property code	Value	Unit	Source
gf	31.76	kJ/mol	Joback Method
hf	-165.69	kJ/mol	Joback Method
hfus	2.50	kJ/mol	Joback Method
hvap	35.08	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.367		Crippen Method
mcvol	126.810	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
rinpol	916.00		NIST Webbook
rinpol	916.00		NIST Webbook
tb	429.38	K	Joback Method
tc	646.05	K	Joback Method
tf	218.95	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.52	J/mol×K	429.38	Joback Method
cpg	275.87	J/mol×K	465.49	Joback Method
cpg	294.88	J/mol×K	501.60	Joback Method
cpg	312.66	J/mol×K	537.71	Joback Method
cpg	329.32	J/mol×K	573.82	Joback Method
cpg	344.96	J/mol×K	609.93	Joback Method
cpg	359.69	J/mol×K	646.05	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R133087&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

Legend

cpg:	Ideal gas heat capacity
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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