

2,3-Dimethylene-bicyclo[2.2.1]heptane

Inchi:	InChI=1S/C9H12/c1-6-7(2)9-4-3-8(6)5-9/h8-9H,1-5H2
InchiKey:	GUBNJQWOCZEVSJ-UHFFFAOYSA-N
Formula:	C9H12
SMILES:	C=C1C(=C)C2CCC1C2
Mol. weight [g/mol]:	120.19

Physical Properties

Property code	Value	Unit	Source
gf	240.46	kJ/mol	Joback Method
hf	78.83	kJ/mol	Joback Method
hfus	10.92	kJ/mol	Joback Method
hvap	35.94	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.529		Crippen Method
mcvol	107.350	ml/mol	McGowan Method
pc	3231.98	kPa	Joback Method
rinpol	970.00		NIST Webbook
rinpol	970.00		NIST Webbook
ripol	1089.00		NIST Webbook
ripol	1089.00		NIST Webbook
tb	421.39	K	Joback Method
tc	624.51	K	Joback Method
tf	250.91	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.26	J/molxK	421.39	Joback Method
cpg	281.76	J/molxK	590.66	Joback Method
cpg	270.07	J/molxK	556.80	Joback Method
cpg	257.62	J/molxK	522.95	Joback Method
cpg	244.37	J/molxK	489.10	Joback Method
cpg	230.26	J/molxK	455.24	Joback Method

cpg	292.74	J/molxK	624.51	Joback Method
dvisc	0.0005663	Paxs	421.39	Joback Method
dvisc	0.0005696	Paxs	392.98	Joback Method
dvisc	0.0005736	Paxs	364.56	Joback Method
dvisc	0.0005782	Paxs	336.15	Joback Method
dvisc	0.0005838	Paxs	307.74	Joback Method
dvisc	0.0005905	Paxs	279.32	Joback Method
dvisc	0.0005989	Paxs	250.91	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=R246574&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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