

5,5-Dimethylbicyclo[2.2.0]pentane

Inchi:	InChI=1S/C7H12/c1-7(2)5-3-4-6(5)7/h5-6H,3-4H2,1-2H3
InchiKey:	RRXLWLMOBNGNIB-UHFFFAOYSA-N
Formula:	C7H12
SMILES:	CC1(C)C2CCC21
Mol. weight [g/mol]:	96.17
CAS:	71805-64-6

Physical Properties

Property code	Value	Unit	Source
gf	128.46	kJ/mol	Joback Method
hf	-41.15	kJ/mol	Joback Method
hfus	7.03	kJ/mol	Joback Method
hvap	29.37	kJ/mol	Joback Method
log10ws	-1.82		Crippen Method
logp	2.052		Crippen Method
mcvol	87.770	ml/mol	McGowan Method
pc	3704.46	kPa	Joback Method
tb	364.34	K	Joback Method
tc	558.62	K	Joback Method
tf	227.71	K	Joback Method
vc	0.346	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.18	J/molxK	364.34	Joback Method
cpg	178.99	J/molxK	396.72	Joback Method
cpg	193.45	J/molxK	429.10	Joback Method
cpg	206.68	J/molxK	461.48	Joback Method
cpg	218.80	J/molxK	493.86	Joback Method
cpg	229.92	J/molxK	526.24	Joback Method
cpg	240.16	J/molxK	558.62	Joback Method

Sources

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=C71805646&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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