

Pentalene, octahydro-2-methyl-

Other names:	3-methylbicyclo[3.3.0]octane
Inchi:	InChI=1S/C9H16/c1-7-5-8-3-2-4-9(8)6-7/h7-9H,2-6H2,1H3
InchiKey:	OWJYQLKKWIHHLI-UHFFFAOYSA-N
Formula:	C9H16
SMILES:	CC1CC2CCCC2C1
Mol. weight [g/mol]:	124.22
CAS:	3868-64-2

Physical Properties

Property code	Value	Unit	Source
gf	114.49	kJ/mol	Joback Method
hf	-116.15	kJ/mol	Joback Method
hfus	12.21	kJ/mol	Joback Method
hvap	35.49	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.833		Crippen Method
mcvol	115.950	ml/mol	McGowan Method
pc	3069.34	kPa	Joback Method
ripol	1056.00		NIST Webbook
ripol	1056.00		NIST Webbook
tb	422.67	K	Joback Method
tc	629.88	K	Joback Method
tf	215.79	K	Joback Method
vc	0.436	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.34	J/molxK	422.67	Joback Method
cpg	328.59	J/molxK	595.34	Joback Method
cpg	313.20	J/molxK	560.81	Joback Method
cpg	296.83	J/molxK	526.27	Joback Method
cpg	279.43	J/molxK	491.74	Joback Method
cpg	260.95	J/molxK	457.20	Joback Method

cpg	343.05	J/mol×K	629.88	Joback Method
dvisc	0.0004936	Paxs	422.67	Joback Method
dvisc	0.0005263	Paxs	388.19	Joback Method
dvisc	0.0005683	Paxs	353.71	Joback Method
dvisc	0.0006238	Paxs	319.23	Joback Method
dvisc	0.0007004	Paxs	284.75	Joback Method
dvisc	0.0008118	Paxs	250.27	Joback Method
dvisc	0.0009865	Paxs	215.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3868642&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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