Pentalene, octahydro-1-methyl-

Other names: 2-methylbicyclo[3.3.0]octane
Inchi: InChI=1S/C9H16/c1-7-5-6-8-3-2-4-9(7)8/h7-9H,2-6H2,1H3
InchiKey: XWDLMQDCTIPQFS-UHFFFAOYSA-N
Formula: C9H16
SMILES: CC1CCC2CCCC12
Mol. weight [g/mol]: 124.22
CAS: 32273-77-1

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	1031.00		NIST Webbook
tb	422.67	K	Joback Method
tc	629.88	K	Joback Method
tf	215.79	K	Joback Method
vc	0.436	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	241.34	J/mol×K	422.67	Joback Method
cpg	260.95	J/mol×K	457.20	Joback Method
cpg	279.43	J/mol×K	491.74	Joback Method
cpg	296.83	J/mol×K	526.27	Joback Method
cpg	313.20	J/mol×K	560.81	Joback Method
cpg	328.59	J/mol×K	595.34	Joback Method
cpg	343.05	J/mol×K	629.88	Joback Method

dvisc	0.0009865	Pa×s	215.79	Joback Method
dvisc	0.0008118	Pa×s	250.27	Joback Method
dvisc	0.0007004	Pa×s	284.75	Joback Method
dvisc	0.0006238	Pa×s	319.23	Joback Method
dvisc	0.0005683	Pa×s	353.71	Joback Method
dvisc	0.0005263	Pa×s	388.19	Joback Method
dvisc	0.0004936	Pa×s	422.67	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=C32273771&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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