Pentalene, 1,2,3,3a,4,6a-hexahydro-

Other names:	Bicyclo[3.3.0]oct-2-ene
	1,2,3,3a,4,6a-hexahydropentalene
Inchi:	InChI=1S/C8H12/c1-3-7-5-2-6-8(7)4-1/h1,3,7-8H,2,4-6H2
InchiKey:	KEHFJHPSOFFXBO-UHFFFAOYSA-N
Formula:	C8H12
SMILES:	C1=CC2CCCC2C1
Mol. weight [g/mol]:	108.18
CAS:	5549-09-7

Physical Properties

Property code	Value	Unit	Source
gf	143.74	kJ/mol	Joback Method
hf	-17.39	kJ/mol	Joback Method
hfus	9.77	kJ/mol	Joback Method
hvap	33.86	kJ/mol	Joback Method
log10ws	-2.33		Crippen Method
logp	2.363		Crippen Method
mcvol	97.560	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
rinpol	850.00		NIST Webbook
tb	403.62	K	Joback Method
tc	615.80	K	Joback Method
tf	209.52	K	Joback Method
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	185.77	J/mol×K	403.62	Joback Method
cpg	202.83	J/mol×K	438.98	Joback Method
cpg	218.77	J/mol×K	474.35	Joback Method
cpg	233.66	J/mol×K	509.71	Joback Method
cpg	247.55	J/mol×K	545.07	Joback Method
cpg	260.50	J/mol×K	580.43	Joback Method

cpg	272.57	J/mol×K	615.80	Joback Method
dvisc	0.0010286	Pa×s	209.52	Joback Method
dvisc	0.0008159	Pa×s	241.87	Joback Method
dvisc	0.0006835	Pa×s	274.22	Joback Method
dvisc	0.0005944	Pa×s	306.57	Joback Method
dvisc	0.0005308	Pa×s	338.92	Joback Method
dvisc	0.0004835	Pa×s	371.27	Joback Method
dvisc	0.0004471	Pa×s	403.62	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5549097&Units=SI

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
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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