1«alpha»,7«alpha»,8a«beta»-Azulene, 1,2,3,5,6,7,8,8a-octahydro-1,4-dimethyl-7-(1-methy

Inchi: InChI=1S/C15H24/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h12-13,15H,1,5-9H2,2-4

InchiKey: YHAJBLWYOIUHHM-IPYPFGDCSA-N

Formula: C15H24

SMILES: C=C(C)C1CCC(C)=C2CCC(C)C2C1

Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	230.80	kJ/mol	Joback Method
hf	-101.83	kJ/mol	Joback Method
hfus	21.40	kJ/mol	Joback Method
hvap	50.22	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1927.05	kPa	Joback Method
ripol	1711.00		NIST Webbook
ripol	1711.00		NIST Webbook
tb	574.17	K	Joback Method
tc	791.30	K	Joback Method
tf	286.45	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.80	J/mol×K	574.17	Joback Method
cpg	525.03	J/mol×K	610.36	Joback Method
cpg	546.90	J/mol×K	646.55	Joback Method
cpg	567.47	J/mol×K	682.74	Joback Method
cpg	586.78	J/mol×K	718.92	Joback Method
cpg	604.90	J/mol×K	755.11	Joback Method
cpg	621.88	J/mol×K	791.30	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=R643668&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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