1H-Cycloprop[e]azulene, 1a«beta»,2,3,4,4a«beta»,5,6,7b«beta»-octahydro-1

Inchi: InChI=1S/C15H26/c1-9-6-8-12-14(15(12,3)4)13-10(2)5-7-11(9)13/h9-14H,5-8H2,1-4H3/t9

InchiKey: UIDUJXXQMGYOIN-GUDWOMEESA-N

Formula: C15H26

SMILES: CC1CCC2C(C3C(C)CCC13)C2(C)C

Mol. weight [g/mol]: 206.37

Physical Properties

Property code	Value	Unit	Source
gf	197.14	kJ/mol	Joback Method
hf	-212.97	kJ/mol	Joback Method
hfus	22.80	kJ/mol	Joback Method
hvap	46.68	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	4.351		Crippen Method
mcvol	189.630	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
rinpol	1400.00		NIST Webbook
tb	552.92	K	Joback Method
tc	766.34	K	Joback Method
tf	312.53	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.56	J/mol×K	552.92	Joback Method
cpg	549.11	J/mol×K	588.49	Joback Method
cpg	573.07	J/mol×K	624.06	Joback Method
cpg	595.59	J/mol×K	659.63	Joback Method
cpg	616.85	J/mol×K	695.20	Joback Method
cpg	637.00	J/mol×K	730.77	Joback Method
cpg	656.19	J/mol×K	766.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R613231&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume