

1H,3a,7-Methanoazulene-2,3,4,7,8,8a-hexahydro-3R«alpha»,3a«beta»,7«beta»,8a«alpha»

InChI=1S/C15H24/c1-10-7-8-15-9-12(10)14(8,4)13(15)6-5-11(15)2/n7,11-13H,5-6,8-9H2
InChIKey: IRAQOCYXUMOF CW OSFYFW SMSA-N

Formula: C15H24
SMILES: CC1=CCC23CC1C(C)(C)C2CCC3C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	227.40	kJ/mol	Joback Method
hf	-110.74	kJ/mol	Joback Method
hfus	15.19	kJ/mol	Joback Method
hvap	47.10	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.415		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	1397.00		NIST Webbook
rinpol	1397.00		NIST Webbook
tb	566.64	K	Joback Method
tc	792.17	K	Joback Method
tf	358.19	K	Joback Method
vc	0.711	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.55	J/molxK	566.64	Joback Method
cpg	526.55	J/molxK	604.23	Joback Method
cpg	547.97	J/molxK	641.82	Joback Method
cpg	568.10	J/molxK	679.41	Joback Method
cpg	587.25	J/molxK	716.99	Joback Method
cpg	605.70	J/molxK	754.58	Joback Method
cpg	623.74	J/molxK	792.17	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=R586897&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
pc:	Critical Pressure
rin_{pol}:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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