1,4-Methanoazulen-7(1H)-one, octahydro-1,5,5,8a-tetramethyl-

Other names: octahydro-1,5,5,8a-tetramethyl-1,4-methanoazulen-7-(1H)-one

Inchi: InChI=1S/C15H24O/c1-13(2)7-10(16)8-15(4)11-5-6-14(15,3)9-12(11)13/h11-12H,5-9H2,

InchiKey: BMLTXHGGEJNZIS-UHFFFAOYSA-N

Formula: C15H24O

SMILES: CC1(C)CC(=O)CC2(C)C3CCC2(C)CC31

Mol. weight [g/mol]: 220.35

CAS: 65437-70-9

Physical Properties

Property code	Value	Unit	Source
gf	78.99	kJ/mol	Joback Method
hf	-279.51	kJ/mol	Joback Method
hfus	7.57	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-3.86		Crippen Method
logp	3.818		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
tb	630.56	K	Joback Method
tc	875.45	K	Joback Method
tf	437.03	K	Joback Method
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.94	J/mol×K	630.56	Joback Method
cpg	584.99	J/mol×K	671.37	Joback Method
cpg	606.96	J/mol×K	712.19	Joback Method
cpg	628.30	J/mol×K	753.00	Joback Method
cpg	649.46	J/mol×K	793.82	Joback Method
cpg	670.93	J/mol×K	834.63	Joback Method
cpg	693.14	J/mol×K	875.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65437709&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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