

1H-3a,7-Methanoazulene-6-methanol, 2,3,4,7,8,8a-hexahydro-3,8,8-trimethyl-, [3R-(3«alpha»,3a«beta»,7«beta»,8a«alpha»)]-2,3,4,7,8,8a-hexahydro-3,6,8-trimethyl-1H-«alpha»-Cedrenol

Inchi: InChI=1S/C15H24O/c1-10-4-5-13-14(2,3)12-8-15(10,13)7-6-11(12)9-16/h6,10,12-13,16H
InchiKey: FUZABTYGEVJEPT-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC1CCC2C(C)(C)C3CC12CC=C3CO
Mol. weight [g/mol]: 220.35
CAS: 21441-72-5

Physical Properties

Property code	Value	Unit	Source
gf	90.58	kJ/mol	Joback Method
hf	-262.97	kJ/mol	Joback Method
hfus	19.28	kJ/mol	Joback Method
hvap	63.78	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	3.387		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2309.17	kPa	Joback Method
rinpol	1669.10		NIST Webbook
rinpol	1669.10		NIST Webbook
rinpol	1695.00		NIST Webbook
tb	658.82	K	Joback Method
tc	867.61	K	Joback Method
tf	419.01	K	Joback Method
vc	0.730	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.50	J/molxK	658.82	Joback Method
cpg	592.95	J/molxK	693.62	Joback Method
cpg	610.61	J/molxK	728.42	Joback Method

cpg	627.74	J/mol×K	763.22	Joback Method
cpg	644.56	J/mol×K	798.01	Joback Method
cpg	661.31	J/mol×K	832.81	Joback Method
cpg	678.22	J/mol×K	867.61	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21441725&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
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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