

3H-3a,7-Methanoazulene, 2,4,5,6,7,8-hexahydro-1,4,9,9-tetramethyl-, [3aR-(3a«alpha»,4«beta»,7«alpha»)]-

Other names: 3H-3a«beta»,7-Methanoazulene,
Cyperene «alpha», 2,4,5,6,7,8-hexahydro-1,4«alpha»,9,9-tetramethyl-, (-)-

Inchi: InChI=1S/C15H24/c1-10-7-8-15-11(2)5-6-12(9-13(10)15)14(15,3)4/h11-12H,5-9H2,1-4H3
InchiKey: RTBLDXVIGWSICW-UHFFFAOYSA-N
Formula: C15H24
SMILES: CC1=C2CC3CCC(C)C2(CC1)C3(C)C
Mol. weight [g/mol]: 204.35
CAS: 2387-78-2

Physical Properties

Property code	Value	Unit	Source
gf	225.48	kJ/mol	Joback Method
hf	-101.87	kJ/mol	Joback Method
hfus	13.73	kJ/mol	Joback Method
hvap	48.07	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.559		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2153.30	kPa	Joback Method
rinpol	1399.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1379.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1398.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1408.00		NIST Webbook
rinpol	1412.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1398.00		NIST Webbook
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rinpol	1402.00	NIST Webbook
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rinpol	1404.00	NIST Webbook
rinpol	1401.00	NIST Webbook
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rinpol	1399.00	NIST Webbook
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ripol	1532.00		NIST Webbook
ripol	1529.00		NIST Webbook
ripol	1514.00		NIST Webbook
ripol	1525.00		NIST Webbook
ripol	1523.00		NIST Webbook
ripol	1520.00		NIST Webbook
tb	576.29	K	Joback Method
tc	802.89	K	Joback Method
tf	374.95	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.46	J/mol×K	576.29	Joback Method
cpg	525.54	J/mol×K	614.06	Joback Method
cpg	546.15	J/mol×K	651.82	Joback Method
cpg	565.60	J/mol×K	689.59	Joback Method
cpg	584.18	J/mol×K	727.36	Joback Method
cpg	602.19	J/mol×K	765.12	Joback Method
cpg	619.93	J/mol×K	802.89	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=C2387782&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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