

2H-Cyclopropa[a]naphthalen-2-one, 1,1a,4,5,6,7,7a,7b-octahydro-1,1,7,7a-tetramethyl-, (1a«alpha»,7«alpha»,7a«alpha»,7b«alpha»)-

Other names:

2H-Cyclopropa[a]naphthalen-2-one,
1,1a,4,5,6,7,7a,7b-octahydro-1,1,7,7a-tetramethyl-,
Aristolone

Inchi: InChI=1S/C15H22O/c1-9-6-5-7-10-8-11(16)12-13(14(12,2)3)15(9,10)4/h8-9,12-13H,5-7H
InchiKey: UGVIZCBJCSXBCJ-PUZVGVIGSA-N
Formula: C15H22O
SMILES: CC1CCCC2=CC(=O)C3C(C3(C)C)C21C
Mol. weight [g/mol]: 218.33
CAS: 6831-17-0

Physical Properties

Property code	Value	Unit	Source
gf	104.81	kJ/mol	Joback Method
hf	-248.44	kJ/mol	Joback Method
hfus	14.70	kJ/mol	Joback Method
hvap	51.35	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.594		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2187.68	kPa	Joback Method
rinpol	1763.00		NIST Webbook
rinpol	1746.00		NIST Webbook
rinpol	1746.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1775.90		NIST Webbook
rinpol	1787.00		NIST Webbook
rinpol	1775.90		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1723.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1762.00		NIST Webbook
ripol	2284.00		NIST Webbook
ripol	2287.00		NIST Webbook

ripol	2284.00		NIST Webbook
tb	634.46	K	Joback Method
tc	873.09	K	Joback Method
tf	426.41	K	Joback Method
vc	0.718	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.90	J/mol×K	634.46	Joback Method
cpg	564.64	J/mol×K	674.23	Joback Method
cpg	585.28	J/mol×K	714.00	Joback Method
cpg	605.11	J/mol×K	753.77	Joback Method
cpg	624.46	J/mol×K	793.54	Joback Method
cpg	643.61	J/mol×K	833.32	Joback Method
cpg	662.89	J/mol×K	873.09	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6831170&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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