

2H-2a,7-Methanoazuleno[5,6-b]oxirene, octahydro-3,6,6,7a-tetramethyl-

Other names:

«alpha»-Cedrene epoxide

«alpha»-Cedrene oxide

«alpha»-Cedren epoxide

NSC 371728

Cedrane, 8,9-epoxide

octahydro-3,6,6,7a-tetramethyl-2H-2a,7-methanoazuleno[5,6-b]oxirene

Inchi:

InChI=1S/C15H24O/c1-9-5-6-10-13(2,3)11-7-15(9,10)8-12-14(11,4)16-12/h9-12H,5-8H2,

InchiKey:

HZRFVTRTTXBHSE-UHFFFAOYSA-N

Formula:

C15H24O

SMILES:

CC1CCC2C(C)(C)C3CC12CC1OC13C

Mol. weight [g/mol]:

220.35

CAS:

29597-36-2

Physical Properties

Property code	Value	Unit	Source
gf	192.70	kJ/mol	Joback Method
hf	-209.03	kJ/mol	Joback Method
hfus	19.44	kJ/mol	Joback Method
hvap	48.77	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.626		Crippen Method
mcvol	184.640	ml/mol	McGowan Method
pc	2244.00	kPa	Joback Method
rinpol	1585.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1568.70		NIST Webbook
rinpol	1570.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1585.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1585.00		NIST Webbook
ripol	1961.00		NIST Webbook
ripol	1961.00		NIST Webbook
ripol	2007.00		NIST Webbook

ripol	1961.00		NIST Webbook
ripol	1978.00		NIST Webbook
ripol	1978.00		NIST Webbook
ripol	2007.00		NIST Webbook
tb	583.22	K	Joback Method
tc	812.69	K	Joback Method
tf	416.12	K	Joback Method
vc	0.716	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.98	J/mol×K	583.22	Joback Method
cpg	563.50	J/mol×K	621.46	Joback Method
cpg	584.43	J/mol×K	659.71	Joback Method
cpg	604.21	J/mol×K	697.95	Joback Method
cpg	623.32	J/mol×K	736.20	Joback Method
cpg	642.20	J/mol×K	774.44	Joback Method
cpg	661.33	J/mol×K	812.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29597362&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
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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