«alpha»-Himachalene

Other names: 1H-Benzocycloheptene, 2,4a«alpha»,5,6,7,8,9,9a«alpha»-octahydro-3,5,5-trimethyl-9-methylene-
1H-Benzocycloheptene, 2,4a,5,6,7,8,9,9a-octahydro-3,5,5-trimethyl-9-methylene-, cis-
1H-Benzocycloheptene, 2,4a,5,6,7,8,9,9a-octahydro-3,5,5-trimethyl-9-methylene-, (4aS,cis)-

Inchi: InChI=1S/C15H24/c1-11-7-8-13-12(2)6-5-9-15(3,4)14(13)10-11/h10,13-14H,2,5-9H2,1,3-

InchiKey: ZJSIKVDEOWWVEH-UHFFFAOYSA-N

Formula: C15H24

SMILES: C=C1CCCC(C)(C)C2C=C(C)CCC12

Mol. weight [g/mol]: 204.36

CAS: 3853-83-6

Physical Properties

Property code	Value	Unit	Source
hf	-76.20	kJ/mol	Cheméo Relay (1.0)
hfus	14.82	kJ/mol	Joback Method
hvap	64.22	kJ/mol	Cheméo Relay (1.0)
ie	8.41	eV	Cheméo Relay (1.0)
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
rinpol	1475.30		NIST Webbook
rinpol	1444.00		NIST Webbook
rinpol	1455.00		NIST Webbook
rinpol	1428.00		NIST Webbook
rinpol	1450.00		NIST Webbook
rinpol	1427.00		NIST Webbook
rinpol	1449.00		NIST Webbook
rinpol	1433.00		NIST Webbook
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ripol	1704.00		NIST Webbook
ripol	1661.00		NIST Webbook
ripol	1684.00		NIST Webbook
ripol	1662.00		NIST Webbook
ripol	1661.00		NIST Webbook
ripol	1655.00		NIST Webbook
ripol	1649.00		NIST Webbook
ripol	1632.00		NIST Webbook
tb	539.98	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-1.36520e+02
Coeff. B	1.71506e+00
Coeff. C	-1.30564e-03
Coeff. D	4.36400e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3853836&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature

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