1H-Benzocycloheptene, 2,4a,5,6,7,8-hexahydro-3,5,5,9-tetramethyl-, (R)-

Other names: «beta»-Himachalene
1H-Benzocycloheptene, 2,4a«beta»,5,6,7,8-hexahydro-3,5,5,9-tetramethyl-, (+)-
(+)-«beta»-Himachalene
3,5,5,9-Tetramethyl-2,4a,5,6,7,8-hexahydro-1H-benzo[a]cycloheptene-, (R)-
1H-Benzocycloheptene, 2,4a,5,6,7,8-hexahydro-3,5,5,9-tetramethyl-, (4aR)-
Himachalene

Inchi: InChI=1S/C15H24/c1-11-7-8-13-12(2)6-5-9-15(3,4)14(13)10-11/h10,14H,5-9H2,1-4H3/t1

InchiKey: LCOSCMLXPAQCLQ-CQSZACIVSA-N

Formula: C15H24

SMILES: CC1=CC2C(=C(C)CCCC2(C)C)CC1

Mol. weight [g/mol]: 204.35

CAS: 1461-03-6

Physical Properties

Property code	Value	Unit	Source
gf	161.96	kJ/mol	Joback Method
hf	-141.74	kJ/mol	Joback Method
hfus	15.35	kJ/mol	Joback Method
hvap	51.09	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	4.869		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	1517.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1499.00		NIST Webbook
rinpol	1503.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1497.00		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1490.00		NIST Webbook
rinpol	1495.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1499.00		NIST Webbook

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rinpol	1498.50	NIST Webbook
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ripol	1711.00	NIST Webbook
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ripol	1715.00	NIST Webbook
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ripol	1742.00	NIST Webbook
ripol	1729.00	NIST Webbook

ripol	1715.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1736.00		NIST Webbook
ripol	1718.00		NIST Webbook
tb	590.93	K	Joback Method
tc	818.95	K	Joback Method
tf	340.07	K	Joback Method
vc	0.720	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	502.99	J/mol×K	590.93	Joback Method
cpg	525.43	J/mol×K	628.93	Joback Method
cpg	546.54	J/mol×K	666.94	Joback Method
cpg	566.46	J/mol×K	704.94	Joback Method
cpg	585.34	J/mol×K	742.94	Joback Method
cpg	603.34	J/mol×K	780.94	Joback Method
cpg	620.59	J/mol×K	818.95	Joback Method

Sources

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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