1H-3a,7-Methanoazulene, octahydro-3,8,8-trimethyl-6-methylene-, [3R-(3«alpha»,3a«beta»,7«beta»,8a«alpha»)]-

Other names: Cedr-8(15)-ene
«beta»-Cedrene
(+)-«beta»-Cedrene
[3R-(3«alpha»,3a«beta»,7«beta»,8a«alpha»)]-octahydro-3,8,8-trimethyl-6-methylene-1H-
Inchi: InChI=1S/C15H24/c1-10-7-8-15-9-12(10)14(3,4)13(15)6-5-11(15)2/h11-13H,1,5-9H2,2-4
InchiKey: DYLPEFGBWGEFBB-KYEXWDHISA-N
Formula: C15H24
SMILES: C=C1CCC23CC1C(C)(C)C2CCC3C
Mol. weight [g/mol]: 204.35
CAS: 546-28-1

Physical Properties

Property code	Value	Unit	Source
gf	260.15	kJ/mol	Joback Method
hf	-72.81	kJ/mol	Joback Method
hfus	13.20	kJ/mol	Joback Method
hvap	46.31	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.415		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinpol	1418.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1420.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1424.00		NIST Webbook
rinpol	1422.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1421.00		NIST Webbook
rinpol	1413.00		NIST Webbook
rinpol	1435.00		NIST Webbook
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rinpol	1422.00		NIST Webbook

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ripol	1633.00		NIST Webbook
ripol	1613.00		NIST Webbook
ripol	1586.00		NIST Webbook
ripol	1633.00		NIST Webbook
ripol	1648.00		NIST Webbook
ripol	1605.00		NIST Webbook
ripol	1638.00		NIST Webbook
ripol	1573.00		NIST Webbook
ripol	1599.00		NIST Webbook
tb	561.66	K	Joback Method
tc	785.91	K	Joback Method
tf	358.59	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.94	J/mol×K	561.66	Joback Method
cpg	525.20	J/mol×K	599.03	Joback Method
cpg	546.85	J/mol×K	636.41	Joback Method
cpg	567.18	J/mol×K	673.78	Joback Method
cpg	586.48	J/mol×K	711.16	Joback Method
cpg	605.02	J/mol×K	748.53	Joback Method
cpg	623.10	J/mol×K	785.91	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C546281&Units=SI

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