Azulene, 1,2,3,3a,4,5,6,7-octahydro-1,4-dimethyl-7-(1-methy
[1R-(1«alpha»,3a«beta»,4«alpha»,7«beta»)]-

Other names: 1«beta»,4«beta»H,10«beta»H-Guaia-5,11-diene
«gamma»-Gurjunene
[1R-(1«alpha»,3a«beta»,4«alpha»,7«beta»)]-1,2,3,3a,4,5,6,7-octahydro-7-isopropenyl-1,
Inchi: InChI=1S/C15H24/c1-10(2)13-7-5-11(3)14-8-6-12(4)15(14)9-13/h9,11-14H,1,5-8H2,2-4H
InchiKey: DUYRYUZIBGFLDD-UHFFFAOYSA-N
Formula: C15H24
SMILES: C=C(C)C1C=C2C(C)CCC2C(C)CC1
Mol. weight [g/mol]: 204.35
CAS: 22567-17-5

Physical Properties

Property code	Value	Unit	Source
gf	232.72	kJ/mol	Joback Method
hf	-110.70	kJ/mol	Joback Method
hfus	22.86	kJ/mol	Joback Method
hvap	49.24	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	4.581		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	1475.00		NIST Webbook
rinpol	1472.00		NIST Webbook
rinpol	1463.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1477.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1473.00		NIST Webbook
rinpol	1475.00		NIST Webbook
rinpol	1471.00		NIST Webbook
rinpol	1476.80		NIST Webbook
rinpol	1469.00		NIST Webbook

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ripol	1676.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1700.00		NIST Webbook
ripol	1647.00		NIST Webbook
tb	564.52	K	Joback Method
tc	780.55	K	Joback Method
tf	269.69	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.34	J/mol×K	564.52	Joback Method
cpg	525.40	J/mol×K	600.53	Joback Method
cpg	548.06	J/mol×K	636.53	Joback Method
cpg	569.37	J/mol×K	672.54	Joback Method
cpg	589.37	J/mol×K	708.54	Joback Method
cpg	608.13	J/mol×K	744.55	Joback Method
cpg	625.69	J/mol×K	780.55	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=C22567175&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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