(3R,3aR,7R,8aS)-3,8,8-Trimethyl-6-methyleneoctal

Other names: 1H-3a,7-Methanoazulene, octahydro-3,8,8-trimethyl-6-methylene-, (3R,3aR,7R,8aS)-
1H-3a,7-Methanoazulene, octahydro-3,8,8-trimethyl-6-methylene-, [3R-(3«alpha»,3a«alpha»,7«alpha»,8a«alpha»)]-
1,7-Di-epi-«beta»-cedrene
«beta»-Funebrene

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-CZPDGURSSA-N

Formula: C15H24

SMILES: C=C1CCC23CC1C(C)(C)C2CCC3C

Mol. weight [g/mol]: 204.35

CAS: 79120-98-2

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	1422.00		NIST Webbook
rinpol	1401.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1434.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1423.00		NIST Webbook
rinpol	1416.00		NIST Webbook
rinpol	1392.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1414.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1404.00		NIST Webbook
rinpol	1415.00		NIST Webbook

rinpol	1413.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1397.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1409.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1409.00		NIST Webbook
ripol	1569.00		NIST Webbook
ripol	1591.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1587.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1618.00		NIST Webbook
ripol	1588.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C79120982&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