5-Azulenemethanol, 1,2,3,4,5,6,7,8-octahydro-«alpha»,«alpha»,3,8-tetra acetate, [3S-(3«alpha», 5«alpha», 8«alpha»)]-

Other names: 5-Azulenemethanol, 1,2,3,4,5,6,7,8-octahydro-«alpha»,«alpha»,3,8-tetramethyl-, G(Al-175)-en-11-ol, acetate
Guaiac acetate
Guaiol acetate
Guaiyl acetate
3,8-Dimethyl-5-alpha-hydroxy-deltadimethyl9-octa hydroazulene acetate
3,8-Dimethyl-5-alpha-hydroxy-delta^9-octa hydroazulene acetate
Guaijol, acetate
3,8-Dimethyl-5-alpha-hydroxy-delta9-octa hydroazulene acetate
1-methyl-1-((3S,8S)-1,2,3,4,5,6,7,8-octahydro-3,8-dimethylazulen-5-yl)ethyl acetate

Inchi: InChI=1S/C17H28O2/c1-11-6-8-14(17(4,5)19-13(3)18)10-16-12(2)7-9-15(11)16/h11-12,1

InchiKey: DRFSOBZVMGLICQ-SGMGOOAPSA-N

Formula: C17H28O2

SMILES: CC(=O)OC(C)(C)C1CCC(C)C2=C(C1)C(C)CC2

Mol. weight [g/mol]: 264.40

CAS: 134-28-1

Physical Properties

Property code	Value	Unit	Source
gf	-62.73	kJ/mol	Joback Method
hf	-512.30	kJ/mol	Joback Method
hfus	24.54	kJ/mol	Joback Method
hvap	63.12	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.491		Crippen Method
mcvol	231.810	ml/mol	McGowan Method
pc	1663.26	kPa	Joback Method
rinpol	1726.00		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1735.00		NIST Webbook
rinpol	1724.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1727.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1714.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1714.00		NIST Webbook

rinpol	1735.00		NIST Webbook
rinpol	1712.00		NIST Webbook
tb	696.43	K	Joback Method
tc	914.62	K	Joback Method
tf	399.29	K	Joback Method
vc	0.868	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	697.93	J/mol×K	696.43	Joback Method
cpg	719.94	J/mol×K	732.80	Joback Method
cpg	740.52	J/mol×K	769.16	Joback Method
cpg	759.70	J/mol×K	805.53	Joback Method
cpg	777.56	J/mol×K	841.89	Joback Method
cpg	794.15	J/mol×K	878.26	Joback Method
cpg	809.53	J/mol×K	914.62	Joback Method
dvisc	0.0018116	Pa×s	399.29	Joback Method
dvisc	0.0010728	Pa×s	448.81	Joback Method
dvisc	0.0007051	Pa×s	498.34	Joback Method
dvisc	0.0004999	Pa×s	547.86	Joback Method
dvisc	0.0003752	Pa×s	597.38	Joback Method
dvisc	0.0002943	Pa×s	646.91	Joback Method
dvisc	0.0002389	Pa×s	696.43	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=C134281&Units=SI

Legend

cpg: Ideal gas heat capacity

dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume