

3,8-Dimethyl-5-alpha-hydroxy-delta9-octahydroazulene acetate

Other names:	5-Azulenemethanol, 1,2,3,4,5«alpha»,6,7,8-octahydro-«alpha»,«alpha»,3«beta»,8«beta»-tetramethyl-, Guaiol-1(5)-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)[C@H]1CC[C@@H](C)C2=C(C1)[C@H](C)CC2
Mol. weight [g/mol]:	264.41

Physical Properties

Property code	Value	Unit	Source
hfus	24.54	kJ/mol	Joback Method
logp	4.491		Crippen Method
mcvol	231.810	ml/mol	McGowan 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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C134281&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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