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

Other names: Guai-1(10)-en-11-ol, Bulnesol

Inchi: InChI=1S/C15H26O/c1-10-5-7-12(15(3,4)16)9-14-11(2)6-8-13(10)14/h11-12,14,16H,5-9H

InchiKey: LGOFSGDSFQNIAT-BZPMIXESSA-N

Formula: C15H26O

SMILES: CC1=C2CCC(C)C2CC(C(C)(C)O)CC1

Mol. weight [g/mol]: 222.37

CAS: 22451-73-6

Physical Properties

Property code	Value	Unit	Source
gf	17.53	kJ/mol	Joback Method
hf	-378.45	kJ/mol	Joback Method
hfus	20.67	kJ/mol	Joback Method
hvap	66.19	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2040.07	kPa	Joback Method
rinpol	1648.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1655.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1652.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1669.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1672.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1664.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1666.00		NIST Webbook

rinpol	1675.00	NIST Webbook
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ripol	2171.00		NIST Webbook
ripol	2202.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2190.00		NIST Webbook
ripol	2180.00		NIST Webbook
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ripol	2204.00		NIST Webbook
ripol	2198.00		NIST Webbook
ripol	2171.00		NIST Webbook
ripol	2225.00		NIST Webbook
ripol	2248.00		NIST Webbook
ripol	2248.00		NIST Webbook
ripol	2204.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2207.00		NIST Webbook
tb	666.56	K	Joback Method
tc	872.62	K	Joback Method
tf	365.41	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.73	J/mol×K	666.56	Joback Method
cpg	621.49	J/mol×K	700.90	Joback Method
cpg	640.04	J/mol×K	735.25	Joback Method
cpg	657.45	J/mol×K	769.59	Joback Method
cpg	673.77	J/mol×K	803.93	Joback Method
cpg	689.07	J/mol×K	838.28	Joback Method
cpg	703.40	J/mol×K	872.62	Joback Method
dvisc	0.0042291	Pa×s	365.41	Joback Method

dvisc	0.0015389	Pa×s	415.60	Joback Method
dvisc	0.0006963	Pa×s	465.79	Joback Method
dvisc	0.0003676	Pa×s	515.99	Joback Method
dvisc	0.0002173	Pa×s	566.18	Joback Method
dvisc	0.0001400	Pa×s	616.37	Joback Method
dvisc	0.0000963	Pa×s	666.56	Joback Method

Sources

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=C22451736&Units=SI
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
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