Sobrerol

Other names: p-menth-6-ene-2,8-diol
5-hydroxy-«alpha»,«alpha»,4-trimethylcyclohex-3-ene-1-methanol
Inchi: InChI=1S/C10H18O2/c1-7-4-5-8(6-9(7)11)10(2,3)12/h4,8-9,11-12H,5-6H2,1-3H3
InchiKey: OMDMTHRBGUBUCO-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CC1=CCC(C(C)(C)O)CC1O
Mol. weight [g/mol]: 170.25
CAS: 498-71-5

Physical Properties

Property code	Value	Unit	Source
gf	-200.41	kJ/mol	Joback Method
hf	-482.65	kJ/mol	Joback Method
hfus	16.16	kJ/mol	Joback Method
hvap	70.99	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	1.475		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	1388.40		NIST Webbook
rinpol	1349.00		NIST Webbook
rinpol	1349.00		NIST Webbook
ripol	2334.00		NIST Webbook
ripol	2334.00		NIST Webbook
tb	628.35	K	Joback Method
tc	816.99	K	Joback Method
tf	342.94	K	Joback Method
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.80	J/mol×K	628.35	Joback Method
cpg	474.67	J/mol×K	785.55	Joback Method

cpg	464.09	J/mol×K	754.11	Joback Method
cpg	452.84	J/mol×K	722.67	Joback Method
cpg	440.89	J/mol×K	691.23	Joback Method
cpg	428.23	J/mol×K	659.79	Joback Method
cpg	484.62	J/mol×K	816.99	Joback Method
dvisc	0.0000277	Pa×s	628.35	Joback Method
dvisc	0.0000508	Pa×s	580.78	Joback Method
dvisc	0.0001040	Pa×s	533.21	Joback Method
dvisc	0.0002449	Pa×s	485.64	Joback Method
dvisc	0.0006945	Pa×s	438.08	Joback Method
dvisc	0.0025385	Pa×s	390.51	Joback Method
dvisc	0.0132934	Pa×s	342.94	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=C498715&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume

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