trans-Sobrerol

Other names: p-Menth-6-en-2,8-diol, trans
trans-5-hydroxy-«alpha»,«alpha»,4-trimethylcyclohex-3-ene-1-methanol
(+) 5-Hydroxy-«alpha»,«alpha»,4-trimethyl-3-cyclohexene-1-methanol
(trans-sobrerol)

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/t8-,9+/m

InchiKey: OMDMTHRBGUBUCO-DTWKUNHWSA-N

Formula: C10H18O2

SMILES: CC1=CCC(C(C)(C)O)CC1O

Mol. weight [g/mol]: 170.25

CAS: 42370-41-2

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	1350.00		NIST Webbook
rinpol	1382.00		NIST Webbook
rinpol	1384.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1399.00		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	484.62	J/mol×K	816.99	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	414.80	J/mol×K	628.35	Joback Method
dvisc	0.0132934	Pa×s	342.94	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
hfust	34.39	kJ/mol	404.90	NIST Webbook

Sources

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=C42370412&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hfust: Enthalpy of fusion at a given temperature
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