Dihydro-«beta»-ionol

Other names:	«beta»-dihydroionol
	7,8-dihydro-«beta»-ionol
	4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-3-butan-2-ol (dihydro-«beta»-ionol)
	«alpha»,2,6,6-tetramethylcyclohexene-1-propan-1-ol
Inchi:	InChI=1S/C13H24O/c1-10-6-5-9-13(3,4)12(10)8-7-11(2)14/h11,14H,5-9H2,1-4H3
InchiKey:	VSYLEWGIVLSDIY-UHFFFAOYSA-N
Formula:	C13H24O
SMILES:	CC1=C(CCC(C)O)C(C)(C)CCC1
Mol. weight [g/mol]:	196.33
CAS:	3293-47-8

Physical Properties

Property code	Value	Unit	Source
gf	-51.02	kJ/mol	Joback Method
hf	-364.76	kJ/mol	Joback Method
hfus	15.97	kJ/mol	Joback Method
hvap	61.72	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.674		Crippen Method
mcvol	184.740	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
rinpol	1455.00		NIST Webbook
rinpol	1449.20		NIST Webbook
ripol	1966.00		NIST Webbook
ripol	1926.00		NIST Webbook
ripol	1915.00		NIST Webbook
ripol	1991.00		NIST Webbook
ripol	1936.00		NIST Webbook
ripol	1926.00		NIST Webbook
ripol	1971.00		NIST Webbook
ripol	1976.00		NIST Webbook
ripol	1907.00		NIST Webbook
ripol	1991.00		NIST Webbook
ripol	1977.00		NIST Webbook
tb	617.49	K	Joback Method
tc	810.80	K	Joback Method
tf	339.17	K	Joback Method

vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.96	J/mol×K	617.49	Joback Method
cpg	515.63	J/mol×K	649.71	Joback Method
cpg	531.52	J/mol×K	681.93	Joback Method
cpg	546.71	J/mol×K	714.14	Joback Method
cpg	561.29	J/mol×K	746.36	Joback Method
cpg	575.34	J/mol×K	778.58	Joback Method
cpg	588.95	J/mol×K	810.80	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=C3293478&Units=SI

Legend

cpg:	Ideal gas heat capacity
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