

7-Oxabicyclo[4.1.0]heptan-3-ol, 6-(3-hydroxy-1-butenyl)-1,5,5-trimethyl-

Other names:	7-Oxabicyclo[4.1.0]heptan-3-ol, 6-(3-hydroxy-1-buten-1-yl)-1,5,5-trimethyl-
Inchi:	InChI=1S/C13H22O3/c1-9(14)5-6-13-11(2,3)7-10(15)8-12(13,4)16-13/h5-6,9-10,14-15H,
InchiKey:	BVNCCXWAZAZQNM-AATRIKPKSA-N
Formula:	C13H22O3
SMILES:	CC(O)C=CC12OC1(C)CC(O)CC2(C)C
Mol. weight [g/mol]:	226.31
CAS:	72777-88-9

Physical Properties

Property code	Value	Unit	Source
gf	-145.89	kJ/mol	Joback Method
hf	-491.69	kJ/mol	Joback Method
hfus	19.68	kJ/mol	Joback Method
hvap	77.90	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	1.632		Crippen Method
mcvol	185.620	ml/mol	McGowan Method
pc	2838.39	kPa	Joback Method
rinpol	1674.10		NIST Webbook
tb	721.00	K	Joback Method
tc	919.63	K	Joback Method
tf	459.98	K	Joback Method
vc	0.695	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.95	J/molxK	721.00	Joback Method
cpg	586.37	J/molxK	754.11	Joback Method
cpg	600.86	J/molxK	787.21	Joback Method
cpg	615.69	J/molxK	820.32	Joback Method
cpg	631.11	J/molxK	853.42	Joback Method
cpg	647.40	J/molxK	886.53	Joback Method
cpg	664.82	J/molxK	919.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C72777889&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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