3-Buten-2-ol, 4-(2,2,6-trimethyl-7-oxabicyclo[4.1.0]hept-1-yl)-

Other names: 6-(3-Hydroxy-1-butenyl)-1,5,5-trimethyl-7-oxabicyclo[4.1.0]heptan-3-ol
Inchi: InChI=1S/C13H22O2/c1-10(14)6-9-13-11(2,3)7-5-8-12(13,4)15-13/h6,9-10,14H,5,7-8H2,
InchiKey: LMCSDSFJYOWGRV-RMKNXTFCSA-N
Formula: C13H22O2
SMILES: CC(O)C=CC12OC1(C)CCCC2(C)C
Mol. weight [g/mol]: 210.31
CAS: 51138-08-0

Physical Properties

Property code	Value	Unit	Source
gf	-1.36	kJ/mol	Joback Method
hf	-319.12	kJ/mol	Joback Method
hfus	14.52	kJ/mol	Joback Method
hvap	61.53	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.661		Crippen Method
mcvol	179.750	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	1698.00		NIST Webbook
rinpol	1698.00		NIST Webbook
tb	633.49	K	Joback Method
tc	844.03	K	Joback Method
tf	403.40	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.90	J/mol×K	633.49	Joback Method
cpg	526.71	J/mol×K	668.58	Joback Method
cpg	541.87	J/mol×K	703.67	Joback Method
cpg	556.70	J/mol×K	738.76	Joback Method
cpg	571.51	J/mol×K	773.85	Joback Method
cpg	586.62	J/mol×K	808.94	Joback Method

cpg	602.36	J/mol×K	844.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51138080&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume