Bicyclo[3.1.0]hex-3-en-2-ol, 2-methyl-5-(1-methylethyl)-, (1«alpha»,2«alpha»,5«alpha»)-

Other names: 5-Isopropyl-2-methylbicyclo[3.1.0]hex-3-en-2-ol
Inchi: InChI=1S/C10H16O/c1-7(2)10-5-4-9(3,12)8(10)6-10/h4-5,7-8,11H,6H2,1-3H3
InchiKey: MSEVJTQZWWZGMP-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC(C)C12C=CC(C)(O)C1C2
Mol. weight [g/mol]: 152.23
CAS: 97631-68-0

Physical Properties

Property code	Value	Unit	Source
gf	26.83	kJ/mol	Joback Method
hf	-193.72	kJ/mol	Joback Method
hfus	8.19	kJ/mol	Joback Method
hvap	51.65	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.969		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	1039.00		NIST Webbook
rinpol	1039.00		NIST Webbook
tb	528.39	K	Joback Method
tc	728.63	K	Joback Method
tf	328.48	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.10	J/mol×K	528.39	Joback Method
cpg	349.04	J/mol×K	561.76	Joback Method
cpg	361.87	J/mol×K	595.14	Joback Method
cpg	373.80	J/mol×K	628.51	Joback Method
cpg	385.01	J/mol×K	661.89	Joback Method
cpg	395.72	J/mol×K	695.26	Joback Method

cpg	406.12	J/mol×K	728.63	Joback Method

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=C97631680&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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