

Bicyclo[3.1.0]hexan-3-ol, 4-methyl-1-(1-methylethyl)-, (1«alpha»,3«beta»,4«beta»,5«alpha»)-

Other names: Neoisothujyl alcohol,
1-Isopropyl-4-methylbicyclo[3.1.0]hexan-3-ol-
(1«alpha»,3«beta»,4«beta»,5«alpha»)-
Neoisothujol

Inchi: InChI=1S/C10H18O/c1-6(2)10-4-8(10)7(3)9(11)5-10/h6-9,11H,4-5H2,1-3H3/t7-,8?,9+,10-
InchiKey: DZVXRFMREAADPP-ITRGKUQCSA-N
Formula: C10H18O
SMILES: CC1C(O)CC2(C(C)C)CC12
Mol. weight [g/mol]: 154.25
CAS: 31187-53-8

Physical Properties

Property code	Value	Unit	Source
gf	-5.35	kJ/mol	Joback Method
hf	-287.08	kJ/mol	Joback Method
hfus	14.34	kJ/mol	Joback Method
hvap	52.20	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.049		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	2956.90	kPa	Joback Method
ripol	1694.00		NIST Webbook
ripol	1694.00		NIST Webbook
ripol	1694.00		NIST Webbook
tb	524.32	K	Joback Method
tc	714.97	K	Joback Method
tf	299.58	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.41	J/molxK	524.32	Joback Method
cpg	370.07	J/molxK	556.10	Joback Method
cpg	384.74	J/molxK	587.87	Joback Method

cpg	398.54	J/mol×K	619.65	Joback Method
cpg	411.57	J/mol×K	651.42	Joback Method
cpg	423.94	J/mol×K	683.20	Joback Method
cpg	435.75	J/mol×K	714.97	Joback Method

Sources

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=C31187538&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

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