3-Thujen-2-ol, stereoisomer

Other names: Umbellulol
3-thujen-2-ol
Inchi: InChI=1S/C10H16O/c1-6(2)10-5-8(10)7(3)4-9(10)11/h4,6,8-9,11H,5H2,1-3H3
InchiKey: OJTQGSSVGDYALN-UHFFFAOYSA-N
Formula: C10H16O
SMILES: CC1=CC(O)C2(C(C)C)CC12
Mol. weight [g/mol]: 152.23
CAS: 3310-03-0

Physical Properties

Property code	Value	Unit	Source
gf	22.69	kJ/mol	Joback Method
hf	-220.43	kJ/mol	Joback Method
hfus	14.10	kJ/mol	Joback Method
hvap	53.46	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.969		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	1107.00		NIST Webbook
ripol	1707.00		NIST Webbook
tb	533.13	K	Joback Method
tc	726.81	K	Joback Method
tf	317.10	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.61	J/mol×K	533.13	Joback Method
cpg	349.43	J/mol×K	565.41	Joback Method
cpg	362.34	J/mol×K	597.69	Joback Method
cpg	374.46	J/mol×K	629.97	Joback Method
cpg	385.91	J/mol×K	662.25	Joback Method

cpg	396.80	J/mol×K	694.53	Joback Method
cpg	407.24	J/mol×K	726.81	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=C3310030&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

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