3-pinen-2-ol

Inchi: InChI=1S/C9H14O/c1-9(2)6-3-4-8(10)7(9)5-6/h3-4,6-8,10H,5H2,1-2H3
InchiKey: UBDKJIGEGLXYBJ-UHFFFAOYSA-N
Formula: C9H14O
SMILES: CC1(C)C2C=CC(O)C1C2
Mol. weight [g/mol]: 138.21

Physical Properties

Property code	Value	Unit	Source
gf	6.53	kJ/mol	Joback Method
hf	-209.54	kJ/mol	Joback Method
hfus	14.39	kJ/mol	Joback Method
hvap	50.83	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.579		Crippen Method
mcvol	117.520	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
rinpol	1079.00		NIST Webbook
rinpol	1079.00		NIST Webbook
tb	505.31	K	Joback Method
tc	702.95	K	Joback Method
tf	300.55	K	Joback Method
vc	0.447	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.66	J/mol×K	505.31	Joback Method
cpg	305.05	J/mol×K	538.25	Joback Method
cpg	318.46	J/mol×K	571.19	Joback Method
cpg	330.97	J/mol×K	604.13	Joback Method
cpg	342.71	J/mol×K	637.07	Joback Method
cpg	353.79	J/mol×K	670.01	Joback Method
cpg	364.32	J/mol×K	702.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R405164&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