

trans-Pinen-2-ol

Inchi:	InChI=1S/C10H16O/c1-9(2)7-4-5-10(3,11)8(9)6-7/h4-5,7-8,11H,6H2,1-3H3/t7-,8+,10-/m1
InchiKey:	QBKKSIMANOEXOI-KHQFGBGNSA-N
Formula:	C10H16O
SMILES:	CC1(O)C=CC2CC1C2(C)C
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
gf	9.46	kJ/mol	Joback Method
hf	-214.94	kJ/mol	Joback Method
hfus	10.68	kJ/mol	Joback Method
hvap	51.90	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.969		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3299.15	kPa	Joback Method
rinpol	1115.00		NIST Webbook
tb	528.43	K	Joback Method
tc	731.27	K	Joback Method
tf	335.72	K	Joback Method
vc	0.500	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.25	J/mol×K	528.43	Joback Method
cpg	351.07	J/mol×K	562.24	Joback Method
cpg	364.78	J/mol×K	596.04	Joback Method
cpg	377.57	J/mol×K	629.85	Joback Method
cpg	389.63	J/mol×K	663.66	Joback Method
cpg	401.16	J/mol×K	697.46	Joback Method
cpg	412.35	J/mol×K	731.27	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=R325241&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

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