

Pinene (alpha and beta)

Inchi: InChI=1S/2C10H16/c2*1-7-4-5-8-6-9(7)10(8,2)3/h4,8-9H,5-6H2,1-3H3;8-9H,1,4-6H2,2-3H2
InchiKey: CUZHJZGRKFEZIY-UHFFFAOYSA-N
Formula: C20H32
SMILES: C=C1CCC2CC1C2(C)C.CC1=CCC2CC1C2(C)C
Mol. weight [g/mol]: 272.47

Physical Properties

Property code	Value	Unit	Source
gf	278.57	kJ/mol	Joback Method
hf	-168.52	kJ/mol	Joback Method
hfus	21.75	kJ/mol	Joback Method
hvap	58.60	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.997		Crippen Method
mcvol	251.480	ml/mol	McGowan Method
pc	1488.44	kPa	Joback Method
tb	688.34	K	Joback Method
tc	916.67	K	Joback Method
tf	413.42	K	Joback Method
vc	0.950	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.65	J/molxK	688.34	Joback Method
cpg	794.14	J/molxK	726.40	Joback Method
cpg	819.49	J/molxK	764.45	Joback Method
cpg	843.96	J/molxK	802.51	Joback Method
cpg	867.84	J/molxK	840.56	Joback Method
cpg	891.40	J/molxK	878.62	Joback Method
cpg	914.93	J/molxK	916.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6010558&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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