trans-Sabinol

Inchi: InChI=1S/C9H16O/c1-6(2)9-4-3-8(10)7(9)5-9/h6-8,10H,3-5H2,1-2H3/t7?,8-,9-/m1/s1
InchiKey: PKSXMHCSAJAURT-CFCGPWAMSA-N
Formula: C9H16O
SMILES: CC(C)C12CCC(O)C1C2
Mol. weight [g/mol]: 140.22

Physical Properties

Property code	Value	Unit	Source
gf	-6.06	kJ/mol	Joback Method
hf	-246.10	kJ/mol	Joback Method
hfus	10.67	kJ/mol	Joback Method
hvap	50.28	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	1.803		Crippen Method
mcvol	121.820	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
rinpol	1147.00		NIST Webbook
rinpol	1101.00		NIST Webbook
rinpol	1101.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1137.00		NIST Webbook
ripol	1721.00		NIST Webbook
ripol	1720.00		NIST Webbook
ripol	1721.00		NIST Webbook
tb	506.11	K	Joback Method
tc	699.38	K	Joback Method
tf	292.55	K	Joback Method
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.11	J/mol×K	506.11	Joback Method

cpg	321.78	J/mol×K	538.32	Joback Method
cpg	335.43	J/mol×K	570.53	Joback Method
cpg	348.17	J/mol×K	602.74	Joback Method
cpg	360.13	J/mol×K	634.95	Joback Method
cpg	371.42	J/mol×K	667.17	Joback Method
cpg	382.15	J/mol×K	699.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R610029&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume