

trans-Sabinenehydrate

Inchi: InChI=1S/C10H18O/c1-7(2)10-5-4-9(3,11)8(10)6-10/h7-8,11H,4-6H2,1-3H3/t8?,9-,10-/m
InchiKey: KXSDPILWGMGFJMM-AGROOBSYSA-N
Formula: C10H18O
SMILES: CC(C)C12CCC(C)(O)C1C2
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
gf	-3.13	kJ/mol	Joback Method
hf	-251.50	kJ/mol	Joback Method
hfus	6.97	kJ/mol	Joback Method
hvap	51.36	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.194		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	3224.64	kPa	Joback Method
rinpol	1087.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1098.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1053.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1060.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1102.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1101.00		NIST Webbook
rinpol	1052.00		NIST Webbook

ripol	1096.00		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1474.00		NIST Webbook
tb	529.23	K	Joback Method
tc	727.62	K	Joback Method
tf	327.72	K	Joback Method
vc	0.517	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.14	J/mol×K	529.23	Joback Method
cpg	368.19	J/mol×K	562.29	Joback Method
cpg	382.12	J/mol×K	595.36	Joback Method
cpg	395.11	J/mol×K	628.42	Joback Method
cpg	407.37	J/mol×K	661.49	Joback Method
cpg	419.07	J/mol×K	694.55	Joback Method
cpg	430.42	J/mol×K	727.62	Joback Method

Sources

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=U121973&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀w_s:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mc_{vol}:	McGowan's characteristic volume
p_c:	Critical Pressure
r_{inpol}:	Non-polar retention indices
r_{ipol}:	Polar retention indices
t_b:	Normal Boiling Point Temperature
t_c:	Critical Temperature
t_f:	Normal melting (fusion) point
v_c:	Critical Volume

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