

trans-Sabinol

Other names:	(E)-Sabinol
Inchi:	InChI=1S/C10H16O/c1-6(2)10-4-8(10)7(3)9(11)5-10/h6,8-9,11H,3-5H2,1-2H3/t8-,9+,10+
InchiKey:	MDFQXBNVOAKNAY-UTLUCORTSA-N
Formula:	C10H16O
SMILES:	<chem>C=C1C(O)CC2(C(C)C)CC12</chem>
Mol. weight [g/mol]:	152.23
CAS:	29606-76-6

Physical Properties

Property code	Value	Unit	Source
gf	55.44	kJ/mol	Joback Method
hf	-182.50	kJ/mol	Joback Method
hfus	12.11	kJ/mol	Joback Method
hvap	52.67	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	1.969		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	1140.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1126.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1148.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1140.00		NIST Webbook

rinpol	1129.00	NIST Webbook
rinpol	1120.00	NIST Webbook
rinpol	1158.00	NIST Webbook
rinpol	1134.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1120.00	NIST Webbook
rinpol	1121.00	NIST Webbook
rinpol	1111.00	NIST Webbook
rinpol	1139.00	NIST Webbook
rinpol	1126.00	NIST Webbook
rinpol	1119.00	NIST Webbook
rinpol	1143.00	NIST Webbook
rinpol	1120.00	NIST Webbook
rinpol	1141.00	NIST Webbook
rinpol	1105.00	NIST Webbook
rinpol	1130.00	NIST Webbook
rinpol	1139.00	NIST Webbook
rinpol	1136.00	NIST Webbook
rinpol	1108.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1127.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1121.00	NIST Webbook
rinpol	1105.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1142.00	NIST Webbook
rinpol	1131.00	NIST Webbook
rinpol	1134.00	NIST Webbook
rinpol	1139.00	NIST Webbook
rinpol	1140.00	NIST Webbook
rinpol	1136.00	NIST Webbook
ripol	1720.00	NIST Webbook
ripol	1708.00	NIST Webbook
ripol	1720.00	NIST Webbook
ripol	1710.00	NIST Webbook
ripol	1719.00	NIST Webbook
ripol	1720.00	NIST Webbook
ripol	1720.00	NIST Webbook
ripol	1719.00	NIST Webbook
ripol	1720.00	NIST Webbook
ripol	1720.00	NIST Webbook
ripol	1683.00	NIST Webbook

tb	528.15	K	Joback Method
tc	720.59	K	Joback Method
tf	317.50	K	Joback Method
vc	0.503	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.82	J/mol×K	528.15	Joback Method
cpg	348.84	J/mol×K	560.22	Joback Method
cpg	361.94	J/mol×K	592.30	Joback Method
cpg	374.24	J/mol×K	624.37	Joback Method
cpg	385.85	J/mol×K	656.45	Joback Method
cpg	396.88	J/mol×K	688.52	Joback Method
cpg	407.43	J/mol×K	720.59	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=C29606766&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	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

Latest version available from:

<https://www.cheméo.com/cid/25-231-7/trans-Sabinol.pdf>

Generated by Cheméo on 2024-04-16 21:33:56.439733693 +0000 UTC m=+15592485.360311010.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.