

(S)-linalool

Other names:	(S)-Linalol (S)-3,7-dimethyl-1,6-octadien-3-ol (d) linalool
Inchi:	InChI=1S/C10H18O/c1-5-10(4,11)8-6-7-9(2)3/h5,7,11H,1,6,8H2,2-4H3
InchiKey:	CDOSHBSSFJOMGT-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	C=CC(C)(O)CCC=C(C)C
Mol. weight [g/mol]:	154.25
CAS:	126-90-9

Physical Properties

Property code	Value	Unit	Source
gf	58.85	kJ/mol	Joback Method
hf	-177.85	kJ/mol	Joback Method
hfus	15.94	kJ/mol	Joback Method
hvap	52.61	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.670		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
tb	517.87	K	Joback Method
tc	697.57	K	Joback Method
tf	244.90	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.03	J/mol×K	517.87	Joback Method
cpg	360.38	J/mol×K	547.82	Joback Method
cpg	372.99	J/mol×K	577.77	Joback Method
cpg	384.91	J/mol×K	607.72	Joback Method
cpg	396.18	J/mol×K	637.67	Joback Method
cpg	406.83	J/mol×K	667.62	Joback Method

cpg	416.91	J/mol×K	697.57	Joback Method
hvapt	65.40	kJ/mol	297.00	NIST Webbook
hvapt	52.40	kJ/mol	392.00	NIST Webbook

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=C126909&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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	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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