

7-Octen-1-ol, 3,7-dimethyl-, (S)-

Other names:	«alpha»-Citronellol Rhodinol S-(-)-3,7-Dimethyl-7-octen-1-ol 3,7-Dimethyl-7-octen-1-ol-, (S)- (-)-Rhodinol (S)-3,7-Dimethyl-7-octen-1-ol Rhobinol
Inchi:	InChI=1S/C10H20O/c1-9(2)5-4-6-10(3)7-8-11/h10-11H,1,4-8H2,2-3H3/t10-/m1/s1
InchiKey:	JGQFVRIQXUFPAH-SNVBAGLBSA-N
Formula:	C10H20O
SMILES:	<chem>C=C(C)CCCC(C)CO</chem>
Mol. weight [g/mol]:	156.27
CAS:	6812-78-8

Physical Properties

Property code	Value	Unit	Source
gf	-26.65	kJ/mol	Joback Method
hf	-291.60	kJ/mol	Joback Method
hfus	19.63	kJ/mol	Joback Method
hvap	53.55	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.751		Crippen Method
mcvol	153.330	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
ripol	1214.40		NIST Webbook
ripol	1211.00		NIST Webbook
ripol	1213.00		NIST Webbook
ripol	1211.00		NIST Webbook
ripol	1211.00		NIST Webbook
ripol	1766.60		NIST Webbook
ripol	1768.40		NIST Webbook
ripol	1767.10		NIST Webbook
ripol	1768.40		NIST Webbook
ripol	1766.60		NIST Webbook
tb	516.50	K	Joback Method
tc	683.07	K	Joback Method
tf	232.56	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.93	J/mol×K	516.50	Joback Method
cpg	375.10	J/mol×K	544.26	Joback Method
cpg	387.73	J/mol×K	572.02	Joback Method
cpg	399.82	J/mol×K	599.79	Joback Method
cpg	411.40	J/mol×K	627.55	Joback Method
cpg	422.48	J/mol×K	655.31	Joback Method
cpg	433.08	J/mol×K	683.07	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C6812788&Units=SI

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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature

tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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