

7-Octen-4-ol, 2-methyl-6-methylene-, (S)-

Other names:	7-Octen-4-ol, 2-methyl-6-methylene-, (-)- (S)-(-)-Ipsenol Ipsenol 2-Methyl-6-methylene-7-octen-4-ol
Inchi:	InChI=1S/C10H18O/c1-5-9(4)7-10(11)6-8(2)3/h5,8,10-11H,1,4,6-7H2,2-3H3
InchiKey:	RHAXCOKCIAVHPB-UHFFFAOYSA-N
Formula:	C10H18O
SMILES:	<chem>C=CC(=C)CC(O)CC(C)C</chem>
Mol. weight [g/mol]:	154.25
CAS:	35628-05-8

Physical Properties

Property code	Value	Unit	Source
gf	58.75	kJ/mol	Joback Method
hf	-171.45	kJ/mol	Joback Method
hfus	14.83	kJ/mol	Joback Method
hvap	52.50	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.526		Crippen Method
mcvol	149.030	ml/mol	McGowan Method
pc	2548.19	kPa	Joback Method
rinpol	1097.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1087.00		NIST Webbook
tb	512.74	K	Joback Method
tc	685.52	K	Joback Method
tf	215.80	K	Joback Method
vc	0.566	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.62	J/mol×K	512.74	Joback Method
cpg	356.56	J/mol×K	541.54	Joback Method
cpg	368.90	J/mol×K	570.33	Joback Method
cpg	380.68	J/mol×K	599.13	Joback Method
cpg	391.92	J/mol×K	627.93	Joback Method
cpg	402.63	J/mol×K	656.73	Joback Method
cpg	412.83	J/mol×K	685.52	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=C35628058&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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