

(S)-2,5-Dimethyl-3-vinylhex-4-en-2-ol

Inchi:	InChI=1S/C10H18O/c1-6-9(7-8(2)3)10(4,5)11/h6-7,9,11H,1H2,2-5H3/t9-/m1/s1
InchiKey:	JWGLVEFPXSKNBN-SECBINFHSA-N
Formula:	C10H18O
SMILES:	C=CC(C=C(C)C)C(C)(C)O
Mol. weight [g/mol]:	154.25
CAS:	35671-15-9

Physical Properties

Property code	Value	Unit	Source
gf	56.41	kJ/mol	Joback Method
hf	-183.13	kJ/mol	Joback Method
hfus	12.42	kJ/mol	Joback Method
hvap	52.22	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.526		Crippen Method
mvol	149.030	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1038.70		NIST Webbook
tb	517.43	K	Joback Method
tc	700.79	K	Joback Method
tf	229.90	K	Joback Method
vc	0.559	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.28	J/mol×K	517.43	Joback Method
cpg	360.97	J/mol×K	547.99	Joback Method
cpg	373.89	J/mol×K	578.55	Joback Method
cpg	386.07	J/mol×K	609.11	Joback Method
cpg	397.57	J/mol×K	639.67	Joback Method
cpg	408.42	J/mol×K	670.23	Joback Method
cpg	418.68	J/mol×K	700.79	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=C35671159&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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