

Prop-1-en-1,2-dimethyl-1-ol

Inchi: InChI=1S/C5H10O/c1-4(2)5(3)6/h6H,1-3H3
InchiKey: BZAZNULYLRVMSW-UHFFFAOYSA-N
Formula: C5H10O
SMILES: CC(C)=C(C)[O]
Mol. weight [g/mol]: 86.13
CAS: 34454-78-9

Physical Properties

Property code	Value	Unit	Source
hf	-241.00	kJ/mol	NIST Webbook
ie	8.15	eV	NIST Webbook
log10ws	-6.15		Crippen Method
logp	1.731		Crippen Method
mcvol	80.730	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C34454789&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Legend

hf: Enthalpy of formation at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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<https://www.chemeo.com/cid/23-301-1/Prop-1-en-1-2-dimethyl-1-ol.pdf>

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