

5-Hepten-2-ol, 6-methyl-

Other names:	6-Methyl-5-hepten-2-ol 6-methylhept-5-en-2-ol 2-Methyl-2-hepten-6-ol (.+/-.)-6-Methyl-5-hepten-2-ol Sulcatol NSC 66273 Methylheptenol DL-6-Methyl-5-hepten-2-ol 6-Methylhept-5-en-2-ol (Sulcatol)
Inchi:	InChI=1S/C8H16O/c1-7(2)5-4-6-8(3)9/h5,8-9H,4,6H2,1-3H3
InchiKey:	OHEFFKYKJVVOX-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	CC(C)=CCCC(C)O
Mol. weight [g/mol]:	128.21
CAS:	4630-06-2

Physical Properties

Property code	Value	Unit	Source
gf	-51.11	kJ/mol	Joback Method
hf	-258.53	kJ/mol	Joback Method
hfus	15.93	kJ/mol	Joback Method
hvap	49.73	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.114		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
tb	478.22	K	Joback Method
tc	651.29	K	Joback Method
tf	206.70	K	Joback Method
vc	0.477	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	326.63	J/mol×K	622.45	Joback Method
cpg	273.37	J/mol×K	478.22	Joback Method
cpg	285.03	J/mol×K	507.07	Joback Method
cpg	296.16	J/mol×K	535.91	Joback Method
cpg	306.79	J/mol×K	564.76	Joback Method
cpg	316.94	J/mol×K	593.60	Joback Method
cpg	335.88	J/mol×K	651.29	Joback Method
hvapt	57.00	kJ/mol	381.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	352.00 ± 1.00	K	2.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4630062&Units=SI
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

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

tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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