

2-Methyl-5-octyn-4-ol

Inchi:	InChI=1S/C9H16O/c1-4-5-6-9(10)7-8(2)3/h8-10H,4,7H2,1-3H3
InchiKey:	YBGQRUFRRPFNKW-UHFFFAOYSA-N
Formula:	C9H16O
SMILES:	CCC#CC(O)CC(C)C
Mol. weight [g/mol]:	140.22
CAS:	60657-70-7

Physical Properties

Property code	Value	Unit	Source
gf	86.00	kJ/mol	Joback Method
hf	-119.58	kJ/mol	Joback Method
hfus	19.23	kJ/mol	Joback Method
hvap	53.68	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	1.807		Crippen Method
mcvol	134.940	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
tb	505.62	K	Joback Method
tc	690.89	K	Joback Method
tf	328.11	K	Joback Method
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.75	J/molxK	505.62	Joback Method
cpg	313.95	J/molxK	536.50	Joback Method
cpg	325.63	J/molxK	567.38	Joback Method
cpg	336.80	J/molxK	598.26	Joback Method
cpg	347.47	J/molxK	629.14	Joback Method
cpg	357.67	J/molxK	660.02	Joback Method
cpg	367.39	J/molxK	690.89	Joback Method

Sources

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=C60657707&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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