

1-Heptene, 3-methoxy-

Other names:	Ether, 1-butylallyl methyl
Inchi:	InChI=1S/C8H16O/c1-4-6-7-8(5-2)9-3/h5,8H,2,4,6-7H2,1,3H3
InchiKey:	IAWBTGWBVHANJP-UHFFFAOYSA-N
Formula:	C8H16O
SMILES:	C=CC(CCCC)OC
Mol. weight [g/mol]:	128.21
CAS:	14093-58-4

Physical Properties

Property code	Value	Unit	Source
gf	-3.12	kJ/mol	Joback Method
hf	-220.52	kJ/mol	Joback Method
hfus	12.86	kJ/mol	Joback Method
hvap	34.75	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.378		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2621.78	kPa	Joback Method
tb	401.10	K	Joback Method
tc	572.13	K	Joback Method
tf	185.39	K	Joback Method
vc	0.476	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.26	J/molxK	401.10	Joback Method
cpg	254.78	J/molxK	429.60	Joback Method
cpg	266.86	J/molxK	458.11	Joback Method
cpg	278.52	J/molxK	486.61	Joback Method
cpg	289.76	J/molxK	515.12	Joback Method
cpg	300.58	J/molxK	543.62	Joback Method
cpg	310.99	J/molxK	572.13	Joback Method
dvisc	0.0060092	Paxs	185.39	Joback Method

dvisc	0.0021778	Paxs	221.34	Joback Method
dvisc	0.0010481	Paxs	257.29	Joback Method
dvisc	0.0006035	Paxs	293.25	Joback Method
dvisc	0.0003920	Paxs	329.20	Joback Method
dvisc	0.0002772	Paxs	365.15	Joback Method
dvisc	0.0002086	Paxs	401.10	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=C14093584&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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