

3-Methoxy-4-methylheptane

Other names:	4-Methyl-3-heptanol, methyl ether
Inchi:	InChI=1S/C9H20O/c1-5-7-8(3)9(6-2)10-4/h8-9H,5-7H2,1-4H3
InchiKey:	ZQNMHIOHDFWPBL-UHFFFAOYSA-N
Formula:	C9H20O
SMILES:	CCCC(C)C(CC)OC
Mol. weight [g/mol]:	144.25

Physical Properties

Property code	Value	Unit	Source
gf	-84.98	kJ/mol	Joback Method
hf	-371.87	kJ/mol	Joback Method
hfus	13.21	kJ/mol	Joback Method
hvap	37.26	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.848		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	935.00		NIST Webbook
tb	426.86	K	Joback Method
tc	597.40	K	Joback Method
tf	183.42	K	Joback Method
vc	0.545	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.83	J/molxK	426.86	Joback Method
cpg	313.39	J/molxK	455.28	Joback Method
cpg	327.45	J/molxK	483.71	Joback Method
cpg	341.03	J/molxK	512.13	Joback Method
cpg	354.12	J/molxK	540.55	Joback Method
cpg	366.73	J/molxK	568.97	Joback Method
cpg	378.87	J/molxK	597.40	Joback Method
dvisc	0.0132381	Paxs	183.42	Joback Method

dvisc	0.0034707	Paxs	223.99	Joback Method
dvisc	0.0013720	Paxs	264.57	Joback Method
dvisc	0.0006942	Paxs	305.14	Joback Method
dvisc	0.0004121	Paxs	345.71	Joback Method
dvisc	0.0002730	Paxs	386.29	Joback Method
dvisc	0.0001956	Paxs	426.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375013&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
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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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