4-Methyl-3-heptanol, methyl ether

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]: 144.26

Physical Properties

Property code	Value	Unit	Source
af	0.4011		Cheméo Relay (1.0)
gf	-84.98	kJ/mol	Joback Method
hf	-339.57	kJ/mol	Cheméo Relay (1.0)
hfus	13.21	kJ/mol	Joback Method
hvap	45.99	kJ/mol	Cheméo Relay (1.0)
logp	2.848		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2304.74	kPa	Joback Method
rinpol	935.00		NIST Webbook
tb	421.74	K	Cheméo Relay (1.0)
tc	592.82	K	Cheméo Relay (1.0)
tf	175.58	K	Cheméo Relay (1.0)
vc	0.506	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

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

dvisc	0.0034707	Pa×s	223.99	Joback Method
dvisc	0.0013720	Pa×s	264.57	Joback Method
dvisc	0.0006942	Pa×s	305.14	Joback Method
dvisc	0.0004121	Pa×s	345.71	Joback Method
dvisc	0.0002730	Pa×s	386.29	Joback Method
dvisc	0.0001956	Pa×s	426.86	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375013&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
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
logp: Octanol/Water partition coefficient
mcvol: 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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.