4-Methyl-1-hepten-4-ol

Inchi: InChI=1S/C8H16O/c1-4-6-8(3,9)7-5-2/h4,9H,1,5-7H2,2-3H3
InchiKey: PYKQMQBNPLNLPS-UHFFFAOYSA-N
Formula: C8H16O
SMILES: C=CCC(C)(O)CCC
Mol. weight [g/mol]: 128.21
CAS: 1186-31-8

Physical Properties

Property code	Value	Unit	Source
hfus	11.87	kJ/mol	Joback Method
hvap	54.53	kJ/mol	Cheméo Relay (1.0)
ie	9.40	eV	Cheméo Relay (1.0)
log10ws	-1.07		Cheméo Relay (1.0)
logp	2.114		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
tb	427.91	K	Cheméo Relay (1.0)
tc	610.63	K	Cheméo Relay (1.0)
tf	213.02	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.74	J/mol×K	468.07	Joback Method
cpg	287.71	J/mol×K	496.75	Joback Method
cpg	299.08	J/mol×K	525.43	Joback Method
cpg	309.88	J/mol×K	554.11	Joback Method
cpg	320.13	J/mol×K	582.79	Joback Method
cpg	329.87	J/mol×K	611.47	Joback Method
cpg	339.11	J/mol×K	640.15	Joback Method
dvisc	0.0700944	Pa×s	241.40	Joback Method
dvisc	0.0133473	Pa×s	279.18	Joback Method
dvisc	0.0037740	Pa×s	316.96	Joback Method
dvisc	0.0013966	Pa×s	354.74	Joback Method
dvisc	0.0006258	Pa×s	392.51	Joback Method

dvisc	0.0003229	Pa×s	430.29	Joback Method
dvisc	0.0001854	Pa×s	468.07	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38593e+01
Coeff. B	-3.77935e+03
Coeff. C	-6.68480e+01
Temperature range (K), min.	345.32
Temperature range (K), max.	508.99

Sources

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1186318&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point