6-HEPTEN-1-OL, 2-METHYL-

Other names: 2-Methyl-6-hepten-1-ol
Inchi: InChI=1S/C8H16O/c1-3-4-5-6-8(2)7-9/h3,8-9H,1,4-7H2,2H3
InchiKey: UVGLIWCAMUOQPL-UHFFFAOYSA-N
Formula: C8H16O
SMILES: C=CCCCC(C)CO
Mol. weight [g/mol]: 128.21
CAS: ---

Physical Properties

Property code	Value	Unit	Source
af	0.6101		Cheméo Relay (1.0)
gf	-34.94	kJ/mol	Joback Method
hf	-264.30	kJ/mol	Cheméo Relay (1.0)
hfus	15.76	kJ/mol	Joback Method
hvap	66.56	kJ/mol	Cheméo Relay (1.0)
ie	9.44	eV	Cheméo Relay (1.0)
log10ws	-1.79		Cheméo Relay (1.0)
logp	1.971		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
rinpol	994.00		NIST Webbook
rinpol	994.00		NIST Webbook
ripol	1480.00		NIST Webbook
ripol	1480.00		NIST Webbook
tb	451.55	K	Cheméo Relay (1.0)
tc	638.31	K	Cheméo Relay (1.0)
tf	197.54	K	Cheméo Relay (1.0)
vc	0.427	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.08	J/mol×K	470.86	Joback Method
cpg	284.36	J/mol×K	498.51	Joback Method

cpg	295.19	J/mol×K	526.16	Joback Method
cpg	305.56	J/mol×K	553.81	Joback Method
cpg	315.50	J/mol×K	581.46	Joback Method
cpg	325.02	J/mol×K	609.11	Joback Method
cpg	334.14	J/mol×K	636.76	Joback Method
dvisc	0.1097275	Pa×s	223.98	Joback Method
dvisc	0.0162547	Pa×s	265.13	Joback Method
dvisc	0.0040223	Pa×s	306.27	Joback Method
dvisc	0.0013856	Pa×s	347.42	Joback Method
dvisc	0.0005982	Pa×s	388.57	Joback Method
dvisc	0.0003033	Pa×s	429.71	Joback Method
dvisc	0.0001732	Pa×s	470.86	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46944e+01
Coeff. B	-4.09285e+03
Coeff. C	-6.96280e+01
Temperature range (K), min.	353.72
Temperature range (K), max.	505.83

Sources

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=U132120&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume