4-Methyl-4-heptanol

Other names: 4-Hydroxy-4-methylheptane
Inchi: InChI=1S/C8H18O/c1-4-6-8(3,9)7-5-2/h9H,4-7H2,1-3H3
InchiKey: IQXKGRKRIRMQCQ-UHFFFAOYSA-N
Formula: C8H18O
SMILES: CCCC(C)(O)CCC
Mol. weight [g/mol]: 130.23
CAS: 598-01-6

Physical Properties

Property code	Value	Unit	Source
af	0.6181		Cheméo Relay (1.0)
gf	-117.50	kJ/mol	Joback Method
hf	-392.70	kJ/mol	Cheméo Relay (1.0)
hfus	13.15	kJ/mol	Joback Method
hvap	57.70	kJ/mol	Cheméo Relay (1.0)
ie	9.53	eV	Cheméo Relay (1.0)
log10ws	-1.52		Cheméo Relay (1.0)
logp	2.338		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2844.44	kPa	Joback Method
tb	434.20	K	NIST Webbook
tb	433.95 ± 1.00	K	NIST Webbook
tc	611.64	K	Cheméo Relay (1.0)
tf	244.66	K	Cheméo Relay (1.0)
vc	0.476	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.77	J/mol×K	640.25	Joback Method
cpg	292.85	J/mol×K	471.39	Joback Method
cpg	305.37	J/mol×K	499.53	Joback Method
cpg	317.32	J/mol×K	527.68	Joback Method
cpg	328.71	J/mol×K	555.82	Joback Method

cpg	339.57	J/mol×K	583.96	Joback Method
cpg	349.91	J/mol×K	612.10	Joback Method
cpl	367.40	J/mol×K	298.50	NIST Webbook
dvisc	0.0742698	Pa×s	243.16	Joback Method
dvisc	0.0138116	Pa×s	281.20	Joback Method
dvisc	0.0038351	Pa×s	319.24	Joback Method
dvisc	0.0013989	Pa×s	357.27	Joback Method
dvisc	0.0006196	Pa×s	395.31	Joback Method
dvisc	0.0003166	Pa×s	433.35	Joback Method
dvisc	0.0001803	Pa×s	471.39	Joback Method
hvapt	54.40	kJ/mol	389.00	NIST Webbook
hvapt	54.80	kJ/mol	382.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.20	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53196e+01
Coeff. B	-3.67394e+03
Coeff. C	-9.08800e+01
Temperature range (K), min.	335.29
Temperature range (K), max.	457.98

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=C598016&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
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume