2-Heptanol, 6-methyl-

Other names:	2-Methylheptan-6-ol
	6-Methyl-2-heptanol
	6-methylheptan-2-ol
	NSC 75858
Inchi:	InChI=1S/C8H18O/c1-7(2)5-4-6-8(3)9/h7-9H,4-6H2,1-3H3
InchiKey:	FCOUHTHQYOMLJT-UHFFFAOYSA-N
Formula:	C8H18O
SMILES:	CC(C)CCCC(C)O
Mol. weight [g/mol]:	130.23
CAS:	4730-22-7

Physical Properties

Property code	Value	Unit	Source
gf	-125.22	kJ/mol	Joback Method
hf	-371.24	kJ/mol	Joback Method
hfus	13.52	kJ/mol	Joback Method
hvap	49.31	kJ/mol	Joback Method
log10ws	-2.30		Crippen Method
logp	2.194		Crippen Method
mcvol	129.450	ml/mol	McGowan Method
pc	2835.36	kPa	Joback Method
rinpol	951.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	960.00		NIST Webbook
ripol	1379.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1352.00		NIST Webbook
ripol	1365.00		NIST Webbook
tb	445.65 ± 3.00	K	NIST Webbook
tb	444.65 ± 3.00	K	NIST Webbook
tb	444.70	K	NIST Webbook
tb	444.65 ± 3.00	K	NIST Webbook
tb	444.65 ± 3.00	K	NIST Webbook
tb	446.65 ± 2.00	K	NIST Webbook
tb	444.65 ± 3.00	K	NIST Webbook

tb	444.95 ± 0.50	K	NIST Webbook
tc	639.93	K	Joback Method
tf	212.00 ± 5.00	K	NIST Webbook
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.45	J/mol×K	639.93	Joback Method
cpg	346.54	J/mol×K	612.23	Joback Method
cpg	336.21	J/mol×K	584.53	Joback Method
cpg	325.44	J/mol×K	556.84	Joback Method
cpg	314.22	J/mol×K	529.14	Joback Method
cpg	302.54	J/mol×K	501.44	Joback Method
cpg	290.39	J/mol×K	473.74	Joback Method
cpl	315.10	J/mol×K	298.50	NIST Webbook
dvisc	0.0001609	Pa×s	473.74	Joback Method
dvisc	0.0002977	Pa×s	429.91	Joback Method
dvisc	0.0006333	Pa×s	386.07	Joback Method
dvisc	0.0016351	Pa×s	342.24	Joback Method
dvisc	0.0055777	Pa×s	298.41	Joback Method
dvisc	0.0290327	Pa×s	254.57	Joback Method
dvisc	0.3001577	Pa×s	210.74	Joback Method
hvapt	55.20	kJ/mol	399.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58531e+01
Coeff. B	-4.15750e+03
Coeff. C	-7.49440e+01
Temperature range (K), min.	342.04
Temperature range (K), max.	469.33

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4730227&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
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