4-Heptanol, 4-propyl-

Other names: 4-Propyl-4-heptanol
Inchi: InChI=1S/C10H22O/c1-4-7-10(11,8-5-2)9-6-3/h11H,4-9H2,1-3H3
InchiKey: SJTPBRMACCDJPZ-UHFFFAOYSA-N
Formula: C10H22O
SMILES: CCCC(O)(CCC)CCC
Mol. weight [g/mol]: 158.28
CAS: 2198-72-3

Physical Properties

Property code	Value	Unit	Source
gf	-100.66	kJ/mol	Joback Method
hf	-410.71	kJ/mol	Joback Method
hfus	18.33	kJ/mol	Joback Method
hvap	53.24	kJ/mol	Joback Method
log10ws	-3.38		Crippen Method
logp	3.118		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2340.56	kPa	Joback Method
tb	465.15 ± 4.00	K	NIST Webbook
tb	467.15 ± 4.00	K	NIST Webbook
tc	683.80	K	Joback Method
tf	265.70	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.55	J/mol×K	517.15	Joback Method
cpg	397.63	J/mol×K	544.92	Joback Method
cpg	411.07	J/mol×K	572.70	Joback Method
cpg	423.89	J/mol×K	600.47	Joback Method
cpg	436.13	J/mol×K	628.25	Joback Method
cpg	447.81	J/mol×K	656.02	Joback Method
cpg	458.94	J/mol×K	683.80	Joback Method

cpl	446.60	J/mol×K	298.15	NIST Webbook
dvisc	0.0428890	Pa×s	265.70	Joback Method
dvisc	0.0082611	Pa×s	307.61	Joback Method
dvisc	0.0023619	Pa×s	349.52	Joback Method
dvisc	0.0008829	Pa×s	391.43	Joback Method
dvisc	0.0003993	Pa×s	433.33	Joback Method
dvisc	0.0002077	Pa×s	475.24	Joback Method
dvisc	0.0001201	Pa×s	517.15	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64066e+01
Coeff. B	-4.66971e+03
Coeff. C	-7.10180e+01
Temperature range (K), min.	360.72
Temperature range (K), max.	491.90

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2198723&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

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

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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume