2-propylpentanal

Inchi: InChI=1S/C8H16O/c1-3-5-8(7-9)6-4-2/h7-8H,3-6H2,1-2H3
InchiKey: BAUHZKXBGXCLBO-UHFFFAOYSA-N
Formula: C8H16O
SMILES: CCCC(C=O)CCC
Mol. weight [g/mol]: 128.21
CAS: 18295-59-5

Physical Properties

Property code	Value	Unit	Source
hfus	15.24	kJ/mol	Joback Method
hvap	47.34	kJ/mol	Cheméo Relay (1.0)
ie	9.45	eV	Cheméo Relay (1.0)
log10ws	-2.45		Cheméo Relay (1.0)
logp	2.402		Crippen Method
mcvol	125.150	ml/mol	McGowan Method
tb	428.44	K	Cheméo Relay (1.0)
tf	205.68	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.75	J/mol×K	430.66	Joback Method
cpg	324.51	J/mol×K	605.22	Joback Method
cpg	314.39	J/mol×K	576.13	Joback Method
cpg	303.81	J/mol×K	547.04	Joback Method
cpg	292.77	J/mol×K	517.94	Joback Method
cpg	281.26	J/mol×K	488.85	Joback Method
cpg	269.26	J/mol×K	459.75	Joback Method
dvisc	0.0008686	Pa×s	318.79	Joback Method
dvisc	0.0003026	Pa×s	430.66	Joback Method
dvisc	0.0004023	Pa×s	393.37	Joback Method
dvisc	0.0005678	Pa×s	356.08	Joback Method
dvisc	0.0077983	Pa×s	206.92	Joback Method
dvisc	0.0014872	Pa×s	281.50	Joback Method

dvisc	0.0030008	Pa×s	244.21	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49782e+01
Coeff. B	-3.92905e+03
Coeff. C	-6.15660e+01
Temperature range (K), min.	329.02
Temperature range (K), max.	468.02

Sources

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

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

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

tf: Normal melting (fusion) point