

2-propylhexanoic acid

Inchi:	InChI=1S/C9H18O2/c1-3-5-7-8(6-4-2)9(10)11/h8H,3-7H2,1-2H3,(H,10,11)
InchiKey:	HWXRWNDOEKHFUHL-UHFFFAOYSA-N
Formula:	C9H18O2
SMILES:	CCCCC(CCC)C(=O)O
Mol. weight [g/mol]:	158.24
CAS:	3274-28-0

Physical Properties

Property code	Value	Unit	Source
af	0.7162		Cheméo Relay (1.0)
gf	-243.28	kJ/mol	Joback Method
hf	-583.36	kJ/mol	Cheméo Relay (1.0)
hfus	21.23	kJ/mol	Joback Method
hvap	73.09	kJ/mol	Cheméo Relay (1.0)
ie	9.93	eV	Cheméo Relay (1.0)
log10ws	-2.60		Cheméo Relay (1.0)
logp	2.678		Crippen Method
mcvol	145.110	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
tb	500.93	K	Cheméo Relay (1.0)
tc	685.15	K	Cheméo Relay (1.0)
tf	241.96	K	Cheméo Relay (1.0)
vc	0.519	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.57	J/mol×K	550.93	Joback Method
cpg	419.88	J/mol×K	721.77	Joback Method
cpg	410.35	J/mol×K	693.29	Joback Method
cpg	400.35	J/mol×K	664.82	Joback Method
cpg	389.89	J/mol×K	636.35	Joback Method
cpg	378.95	J/mol×K	607.88	Joback Method
cpg	367.51	J/mol×K	579.40	Joback Method

dvisc	0.0007142	Pa×s	418.93	Joback Method
dvisc	0.0001171	Pa×s	550.93	Joback Method
dvisc	0.0001927	Pa×s	506.93	Joback Method
dvisc	0.0003486	Pa×s	462.93	Joback Method
dvisc	0.0229838	Pa×s	286.94	Joback Method
dvisc	0.0017314	Pa×s	374.94	Joback Method
dvisc	0.0053119	Pa×s	330.94	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.63663e+01
Coeff. B	-5.07619e+03
Coeff. C	-8.75310e+01
Temperature range (K), min.	403.24
Temperature range (K), max.	546.71

Sources

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor
Pressure:
Joback Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

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):

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
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/100-779-6/2-propylhexanoic-acid.pdf>

Generated by Cheméo on 2026-07-21 16:40:56.966309453 +0000 UTC m=+163152.808194832.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.