

4-Propyl-4-heptanol

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

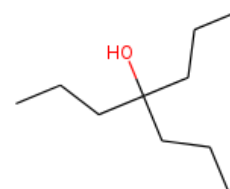
InChI Key: SJTPBRMACCDJPZ-UHFFFAOYSA-N

Formula: C10H22O

SMILES: CCCC(O)(CCC)CCC

Molecular Weight: 158.28

CAS: 2198-72-3



Physical Properties

Property	Value	Unit	Source
$\Delta_f G^\circ$	-100.66	kJ/mol	Joback Method
$\Delta_f H^\circ_{\text{gas}}$	-410.71	kJ/mol	Joback Method
$\Delta_{\text{fus}} H^\circ$	18.33	kJ/mol	Joback Method
$\Delta_{\text{vap}} H^\circ$	53.24	kJ/mol	Joback Method
$\log P_{\text{oct/wat}}$	3.12		Crippen Method
P_c	2340.56	kPa	Joback Method
T_{boil}	467.15 ± 4.00	K	NIST Webbook
T_{boil}	465.15 ± 4.00	K	NIST Webbook
T_c	683.80	K	Joback Method
T_{fus}	265.70	K	Joback Method
V_c	0.60	m ³ /kg-mol	Joback Method

Temperature Dependent Properties

Property	Value	Unit	Temperature (K)	Source
$C_{p,\text{gas}}$	383.55	J/mol×K	517.15	Joback Method
$C_{p,\text{liquid}}$	446.60	J/mol×K	298.15	NIST Webbook

Property	Value	Unit	Temperature (K)	Source
η	0.00	Paxs	517.15	Joback Method

Sources

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

NIST Webbook:

[http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H22O/c1-4-7-10\(11,8-5-2\)9-6-3/h11H,4-9H2,1-3H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C10H22O/c1-4-7-10(11,8-5-2)9-6-3/h11H,4-9H2,1-3H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$C_{p,gas}$: Ideal gas heat capacity (J/mol×K).

$C_{p,liquid}$: Liquid phase heat capacity (J/mol×K).

η : Dynamic viscosity (Paxs).

$\Delta_f G^\circ$: Standard Gibbs free energy of formation (kJ/mol).

$\Delta_f H^\circ_{gas}$: Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{fus} H^\circ$: Enthalpy of fusion at standard conditions (kJ/mol).

$\Delta_{vap} H^\circ$: Enthalpy of vaporization at standard conditions (kJ/mol).

$logP_{oct/wat}$: Octanol/Water partition coefficient .

P_c : Critical Pressure (kPa).

T_{boil} : Normal Boiling Point Temperature (K).

T_c : Critical Temperature (K).

T_{fus} : Normal melting (fusion) point (K).

V_c : Critical Volume (m³/kg-mol).

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