

Isodecanol

Inchi:

InChI=1S/C10H22O/c1-10(2)8-6-4-3-5-7-9-11/h10-11H,3-9H2,1-2H3

InchiKey:

PLLBRTOLHQQAQQ-UHFFFAOYSA-N

Formula:

C10H22O

SMILES:

CC(C)CCCCCCCCO

Mol. weight [g/mol]:

158.29

CAS:

25339-17-7

Physical Properties

Property code	Value	Unit	Source
af	0.7474		Cheméo Relay (1.0)
gf	-105.94	kJ/mol	Joback Method
hf	-423.22	kJ/mol	Cheméo Relay (1.0)
hfus	22.22	kJ/mol	Joback Method
hvap	79.19	kJ/mol	Cheméo Relay (1.0)
ie	9.83	eV	Cheméo Relay (1.0)
log10ws	-3.61		Cheméo Relay (1.0)
logp	2.975		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
tb	502.75	K	Cheméo Relay (1.0)
tc	688.29	K	Cheméo Relay (1.0)
tf	278.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)
vc	0.588	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-2.59300e+00
Coeff. B	9.93740e-01

Coeff. C	-5.53800e-04
Coeff. D	1.17100e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	$Y = \exp(A + B/T + C \cdot \ln(T) + D \cdot T^E)$
Y unit	Pa·s
Coeff. A	-1.48386e+01
Coeff. B	3.00945e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from T_f to $0.7 \cdot T_c$.
Temperature range (K), min.	278.15
Temperature range (K), max.	477.06

Sources

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):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
pc:	Critical 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/107-054-3/Isodecanol.pdf>

Generated by Cheméo on 2026-10-30 23:21:06.257093208 +0000 UTC m=+26179.183930494.

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