4-Undecanol

Other names: undecan-4-ol
Inchi: InChI=1S/C11H24O/c1-3-5-6-7-8-10-11(12)9-4-2/h11-12H,3-10H2,1-2H3
InchiKey: FNORHVDKJWGANC-UHFFFAOYSA-N
Formula: C11H24O
SMILES: CCCCCCCC(O)CCC
Mol. weight [g/mol]: 172.31
CAS: 4272-06-4

Physical Properties

Property code	Value	Unit	Source
af	0.7342		Cheméo Relay (1.0)
gf	-97.52	kJ/mol	Joback Method
hf	-440.78	kJ/mol	Cheméo Relay (1.0)
hfus	24.81	kJ/mol	Joback Method
hvap	80.26	kJ/mol	Cheméo Relay (1.0)
ie	9.69	eV	Cheméo Relay (1.0)
log10ws	-3.59		Cheméo Relay (1.0)
logp	3.508		Crippen Method
mcvol	171.720	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
ripol	1672.00		NIST Webbook
ripol	1648.00		NIST Webbook
ripol	1651.00		NIST Webbook
ripol	1672.00		NIST Webbook
ripol	1682.00		NIST Webbook
ripol	1682.00		NIST Webbook
ripol	1648.00		NIST Webbook
tb	497.30	K	Cheméo Relay (1.0)
tc	678.82	K	Cheméo Relay (1.0)
tf	280.00	K	Cheméo Relay (1.0)
vc	0.671	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.91	J/mol×K	542.82	Joback Method
cpg	506.33	J/mol×K	703.49	Joback Method
cpg	494.72	J/mol×K	676.71	Joback Method
cpg	482.61	J/mol×K	649.93	Joback Method
cpg	469.99	J/mol×K	623.16	Joback Method
cpg	456.84	J/mol×K	596.38	Joback Method
cpg	443.16	J/mol×K	569.60	Joback Method
dvisc	0.0007343	Pa×s	401.18	Joback Method
dvisc	0.0000976	Pa×s	542.82	Joback Method
dvisc	0.0001682	Pa×s	495.61	Joback Method
dvisc	0.0003252	Pa×s	448.40	Joback Method
dvisc	0.0500348	Pa×s	259.55	Joback Method
dvisc	0.0020606	Pa×s	353.97	Joback Method
dvisc	0.0079438	Pa×s	306.76	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60089e+01
Coeff. B	-4.84174e+03
Coeff. C	-8.07480e+01
Temperature range (K), min.	388.72
Temperature range (K), max.	533.35

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4272064&Units=SI

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

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

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
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume