5-Undecanol

Other names: undecan-5-ol
Inchi: InChI=1S/C11H24O/c1-3-5-7-8-10-11(12)9-6-4-2/h11-12H,3-10H2,1-2H3
InchiKey: PCFOZHPCKQPZCN-UHFFFAOYSA-N
Formula: C11H24O
SMILES: CCCCCCC(O)CCCC
Mol. weight [g/mol]: 172.31
CAS: 37493-70-2

Physical Properties

Property code	Value	Unit	Source
af	0.7349		Cheméo Relay (1.0)
gf	-97.52	kJ/mol	Joback Method
hf	-443.90	kJ/mol	Cheméo Relay (1.0)
hfus	24.81	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Cheméo Relay (1.0)
ie	9.73	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
rinpol	1376.00		NIST Webbook
rinpol	1376.00		NIST Webbook
ripol	1671.00		NIST Webbook
ripol	1671.00		NIST Webbook
tb	496.15	K	Cheméo Relay (1.0)
tc	679.69	K	Cheméo Relay (1.0)
tf	280.15	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	443.16	J/mol×K	569.60	Joback Method

cpg	456.84	J/mol×K	596.38	Joback Method
cpg	469.99	J/mol×K	623.16	Joback Method
cpg	482.61	J/mol×K	649.93	Joback Method
cpg	494.72	J/mol×K	676.71	Joback Method
cpg	506.33	J/mol×K	703.49	Joback Method
dvisc	0.0500348	Pa×s	259.55	Joback Method
dvisc	0.0079438	Pa×s	306.76	Joback Method
dvisc	0.0020606	Pa×s	353.97	Joback Method
dvisc	0.0007343	Pa×s	401.18	Joback Method
dvisc	0.0003252	Pa×s	448.40	Joback Method
dvisc	0.0001682	Pa×s	495.61	Joback Method
dvisc	0.0000976	Pa×s	542.82	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

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37493702&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):

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume