

Undecanol-5

Other names:	5-Undecanol 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:	PCFOZHPCCKQPZCN-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
gf	-97.52	kJ/mol	Joback Method
hf	-427.88	kJ/mol	Joback Method
hfus	24.81	kJ/mol	Joback Method
hvap	56.37	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
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	542.82	K	Joback Method
tc	703.49	K	Joback Method
tf	259.55	K	Joback Method
vc	0.664	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.91	J/mol×K	542.82	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
cpg	506.33	J/mol×K	703.49	Joback Method
dvisc	0.0000976	Paxs	542.82	Joback Method
dvisc	0.0001682	Paxs	495.61	Joback Method
dvisc	0.0003252	Paxs	448.40	Joback Method
dvisc	0.0007343	Paxs	401.18	Joback Method
dvisc	0.0020606	Paxs	353.97	Joback Method
dvisc	0.0079438	Paxs	306.76	Joback Method
dvisc	0.0500348	Paxs	259.55	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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=C37493702&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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