2-Undecanol

Other names:	2-Hydroxyundecane
	Methyl nonyl carbinol
	Undecan-2-ol
	Undecylic alcohol, sec-
	sec-Undecyl Alcohol
Inchi:	InChI=1S/C11H24O/c1-3-4-5-6-7-8-9-10-11(2)12/h11-12H,3-10H2,1-2H3
InchiKey:	XMUJIPOFTAHSOK-UHFFFAOYSA-N
Formula:	C11H24O
SMILES:	CCCCCCCCCC(C)O
Mol. weight [g/mol]:	172.31
CAS:	1653-30-1

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	-2.94		Estimated Solubility Method
log10ws	-2.94		Aqueous Solubility Prediction Method
logp	3.508		Crippen Method
mcvol	171.720	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	1285.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1287.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1286.00		NIST Webbook
rinpol	1310.00		NIST Webbook
rinpol	1303.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1311.00		NIST Webbook

rinpol	1298.00		NIST Webbook
rinpol	1270.00		NIST Webbook
rinpol	1285.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1311.00		NIST Webbook
rinpol	1307.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1286.00		NIST Webbook
ripol	1718.00		NIST Webbook
ripol	1704.00		NIST Webbook
ripol	1716.00		NIST Webbook
ripol	1705.00		NIST Webbook
ripol	1726.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1722.00		NIST Webbook
ripol	1722.00		NIST Webbook
ripol	1722.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1726.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1717.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1726.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1717.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1724.00		NIST Webbook
ripol	1710.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1717.00		NIST Webbook
ripol	1738.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1717.00		NIST Webbook
tb	507.15 ± 5.00	K	NIST Webbook
tb	501.15 ± 5.00	K	NIST Webbook
tb	503.15 ± 5.00	K	NIST Webbook
tb	501.65 ± 4.00	K	NIST Webbook
tb	503.65 ± 4.00	K	NIST Webbook
tb	501.15 ± 3.00	K	NIST Webbook

tb	501.15 ± 5.00	K	NIST Webbook
tb	505.15 ± 5.00	K	NIST Webbook
tb	505.15 ± 4.00	K	NIST Webbook
tc	703.49	K	Joback Method
tf	259.55	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.33	J/mol×K	703.49	Joback Method
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
dvisc	0.0000976	Pa×s	542.82	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
hvapt	61.40	kJ/mol	424.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.67068e+01
Coeff. B	-5.09095e+03
Coeff. C	-8.18600e+01
Temperature range (K), min.	391.92
Temperature range (K), max.	528.62

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1653301&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/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

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
hvapt:	Enthalpy of vaporization at a given temperature
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