1-Undecen-3-ol

Other names:	undec-1-en-3-ol
Inchi:	InChI=1S/C11H22O/c1-3-5-6-7-8-9-10-11(12)4-2/h4,11-12H,2-3,5-10H2,1H3
InchiKey:	NAOMHUDQUVEWEF-UHFFFAOYSA-N
Formula:	C11H22O
SMILES:	C=CC(O)CCCCCCCC
Mol. weight [g/mol]:	170.29
CAS:	35329-42-1

Physical Properties

Property code	Value	Unit	Source
gf	-9.68	kJ/mol	Joback Method
hf	-302.45	kJ/mol	Joback Method
hfus	23.53	kJ/mol	Joback Method
hvap	55.70	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.284		Crippen Method
mcvol	167.420	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
rinpol	1293.00		NIST Webbook
rinpol	1293.00		NIST Webbook
tb	539.50	K	Joback Method
tc	702.67	K	Joback Method
tf	257.79	K	Joback Method
vc	0.645	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.38	J/mol×K	539.50	Joback Method
cpg	423.11	J/mol×K	566.69	Joback Method
cpg	436.28	J/mol×K	593.89	Joback Method
cpg	448.90	J/mol×K	621.08	Joback Method
cpg	460.99	J/mol×K	648.28	Joback Method
cpg	472.57	J/mol×K	675.47	Joback Method

cpg	483.65	J/mol×K	702.67	Joback Method
dvisc	0.0477904	Pa×s	257.79	Joback Method
dvisc	0.0077747	Pa×s	304.74	Joback Method
dvisc	0.0020540	Pa×s	351.69	Joback Method
dvisc	0.0007425	Pa×s	398.64	Joback Method
dvisc	0.0003326	Pa×s	445.60	Joback Method
dvisc	0.0001736	Pa×s	492.55	Joback Method
dvisc	0.0001015	Pa×s	539.50	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35329421&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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