

10-Undecyn-1-ol

Inchi:	InChI=1S/C11H20O/c1-2-3-4-5-6-7-8-9-10-11-12/h1,12H,3-11H2
InchiKey:	YUQZOUNRPZBQJK-UHFFFAOYSA-N
Formula:	C11H20O
SMILES:	C#CCCCCCCCCO
Mol. weight [g/mol]:	168.28
CAS:	2774-84-7

Physical Properties

Property code	Value	Unit	Source
gf	127.99	kJ/mol	Joback Method
hf	-130.70	kJ/mol	Joback Method
hfus	31.31	kJ/mol	Joback Method
hvap	56.62	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.733		Crippen Method
mcvol	163.120	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
ripol	2318.00		NIST Webbook
ripol	2318.00		NIST Webbook
tb	533.38	K	Joback Method
tc	699.76	K	Joback Method
tf	321.52	K	Joback Method
vc	0.632	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.90	J/mol×K	533.38	Joback Method
cpg	403.77	J/mol×K	561.11	Joback Method
cpg	416.09	J/mol×K	588.84	Joback Method
cpg	427.90	J/mol×K	616.57	Joback Method
cpg	439.20	J/mol×K	644.30	Joback Method
cpg	450.02	J/mol×K	672.03	Joback Method
cpg	460.37	J/mol×K	699.76	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	384.50 ± 0.50	K	0.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.63479e+01
Coeff. B	-5.26673e+03
Coeff. C	-9.13790e+01
Temperature range (K), min.	419.15
Temperature range (K), max.	568.15

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2774847&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
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:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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