

1-Undecyn-4-ol

Inchi:	InChI=1S/C11H20O/c1-3-5-6-7-8-10-11(12)9-4-2/h2,11-12H,3,5-10H2,1H3
InchiKey:	IBEKWLNDNQDLQS-UHFFFAOYSA-N
Formula:	C11H20O
SMILES:	C#CCC(O)CCCCCCC
Mol. weight [g/mol]:	168.28
CAS:	22127-86-2

Physical Properties

Property code	Value	Unit	Source
gf	125.55	kJ/mol	Joback Method
hf	-135.98	kJ/mol	Joback Method
hfus	27.79	kJ/mol	Joback Method
hvap	56.23	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	2.731		Crippen Method
mcvol	163.120	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	1107.00		NIST Webbook
rinpol	1107.00		NIST Webbook
tb	532.94	K	Joback Method
tc	702.37	K	Joback Method
tf	306.52	K	Joback Method
vc	0.626	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.18	J/mol×K	532.94	Joback Method
cpg	404.34	J/mol×K	561.18	Joback Method
cpg	416.94	J/mol×K	589.42	Joback Method
cpg	428.99	J/mol×K	617.66	Joback Method
cpg	440.51	J/mol×K	645.89	Joback Method
cpg	451.52	J/mol×K	674.13	Joback Method
cpg	462.05	J/mol×K	702.37	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=C22127862&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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