

1-undecenone-5

Inchi:	InChI=1S/C11H20O/c1-3-5-7-8-10-11(12)9-6-4-2/h4H,2-3,5-10H2,1H3
InchiKey:	JNPDGURVXCOKCA-UHFFFAOYSA-N
Formula:	C11H20O
SMILES:	C=CCCC(=O)CCCCC
Mol. weight [g/mol]:	168.28

Physical Properties

Property code	Value	Unit	Source
gf	0.66	kJ/mol	Joback Method
hf	-257.52	kJ/mol	Joback Method
hfus	24.57	kJ/mol	Joback Method
hvap	46.16	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.492		Crippen Method
mcvol	163.120	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
ripol	1569.00		NIST Webbook
ripol	1569.00		NIST Webbook
tb	501.63	K	Joback Method
tc	676.25	K	Joback Method
tf	261.90	K	Joback Method
vc	0.638	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.82	J/molxK	501.63	Joback Method
cpg	384.53	J/molxK	530.73	Joback Method
cpg	398.62	J/molxK	559.84	Joback Method
cpg	412.08	J/molxK	588.94	Joback Method
cpg	424.95	J/molxK	618.04	Joback Method
cpg	437.24	J/molxK	647.14	Joback Method
cpg	448.97	J/molxK	676.25	Joback Method
dvisc	0.0041360	Paxs	261.90	Joback Method

dvisc	0.0019115	Paxs	301.85	Joback Method
dvisc	0.0010581	Paxs	341.81	Joback Method
dvisc	0.0006629	Paxs	381.76	Joback Method
dvisc	0.0004538	Paxs	421.72	Joback Method
dvisc	0.0003317	Paxs	461.68	Joback Method
dvisc	0.0002548	Paxs	501.63	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=R327054&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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