

Undecane, 3,9-dimethyl-

Other names:	3,9-Dimethylundecane
Inchi:	InChI=1S/C13H28/c1-5-12(3)10-8-7-9-11-13(4)6-2/h12-13H,5-11H2,1-4H3
InchiKey:	HHEVJJIJTUVLTQ-UHFFFAOYSA-N
Formula:	C13H28
SMILES:	CCC(C)CCCCC(C)CC
Mol. weight [g/mol]:	184.36
CAS:	17301-31-4

Physical Properties

Property code	Value	Unit	Source
gf	53.70	kJ/mol	Joback Method
hf	-322.21	kJ/mol	Joback Method
hfus	22.38	kJ/mol	Joback Method
hvap	43.76	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	5.029		Crippen Method
mcvol	194.030	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
rinpol	1239.00		NIST Webbook
rinpol	1242.00		NIST Webbook
rinpol	1241.00		NIST Webbook
rinpol	1238.00		NIST Webbook
tb	495.96	K	Joback Method
tc	662.44	K	Joback Method
tf	206.27	K	Joback Method
vc	0.751	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	455.70	J/molxK	495.96	Joback Method
cpg	473.97	J/molxK	523.71	Joback Method
cpg	491.53	J/molxK	551.45	Joback Method
cpg	508.38	J/molxK	579.20	Joback Method

cpg	524.55	J/mol×K	606.95	Joback Method
cpg	540.06	J/mol×K	634.69	Joback Method
cpg	554.93	J/mol×K	662.44	Joback Method
dvisc	0.0170093	Paxs	206.27	Joback Method
dvisc	0.0038696	Paxs	254.55	Joback Method
dvisc	0.0014115	Paxs	302.83	Joback Method
dvisc	0.0006795	Paxs	351.12	Joback Method
dvisc	0.0003903	Paxs	399.40	Joback Method
dvisc	0.0002527	Paxs	447.68	Joback Method
dvisc	0.0001780	Paxs	495.96	Joback Method

Sources

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=C17301314&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
mvol:	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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