

Undecane, 3,6-dimethyl-

Other names:	3,6-Dimethylundecane
Inchi:	InChI=1S/C13H28/c1-5-7-8-9-13(4)11-10-12(3)6-2/h12-13H,5-11H2,1-4H3
InchiKey:	WLUQEGDKTQZXBV-UHFFFAOYSA-N
Formula:	C13H28
SMILES:	CCCCC(C)CCC(C)CC
Mol. weight [g/mol]:	184.36
CAS:	17301-28-9

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
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/mol×K	495.96	Joback Method
cpg	540.06	J/mol×K	634.69	Joback Method
cpg	524.55	J/mol×K	606.95	Joback Method
cpg	508.38	J/mol×K	579.20	Joback Method
cpg	491.53	J/mol×K	551.45	Joback Method
cpg	473.97	J/mol×K	523.71	Joback Method
cpg	554.93	J/mol×K	662.44	Joback Method
dvisc	0.0001780	Pa×s	495.96	Joback Method

dvisc	0.0002527	Pa×s	447.68	Joback Method
dvisc	0.0003903	Pa×s	399.40	Joback Method
dvisc	0.0006795	Pa×s	351.12	Joback Method
dvisc	0.0014115	Pa×s	302.83	Joback Method
dvisc	0.0038696	Pa×s	254.55	Joback Method
dvisc	0.0170093	Pa×s	206.27	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=C17301289&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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