

Undecane, 2,3-dimethyl-

Other names:	2,3-Dimethylundecane
Inchi:	InChI=1S/C13H28/c1-5-6-7-8-9-10-11-13(4)12(2)3/h12-13H,5-11H2,1-4H3
InchiKey:	QSSUTSOGIQHRIU-UHFFFAOYSA-N
Formula:	C13H28
SMILES:	CCCCCCCCC(C)C(C)C
Mol. weight [g/mol]:	184.36
CAS:	17312-77-5

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	1251.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1251.40		NIST Webbook
rinpol	1251.00		NIST Webbook
rinpol	1234.00		NIST Webbook
tb	495.96	K	Joback Method
tc	662.44	K	Joback Method
tf	206.27	K	Joback Method
vc	0.751	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	554.93	J/molxK	662.44	Joback Method
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/molxK	606.95	Joback Method
cpg	540.06	J/molxK	634.69	Joback Method
dvisc	0.0001780	Paxs	495.96	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
hvapt	53.20	kJ/mol	441.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.41125e+01
Coeff. B	-3.81876e+03
Coeff. C	-9.89300e+01
Temperature range (K), min.	375.15
Temperature range (K), max.	532.83

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=C17312775&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

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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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