

3-Ethyl-3-methyl-undecane

Inchi:	InChI=1S/C14H30/c1-5-8-9-10-11-12-13-14(4,6-2)7-3/h5-13H2,1-4H3
InchiKey:	CYOLZLXWAGKBLQ-UHFFFAOYSA-N
Formula:	C14H30
SMILES:	CCCCCCCC(C)(CC)CC
Mol. weight [g/mol]:	198.39

Physical Properties

Property code	Value	Unit	Source
gf	69.84	kJ/mol	Joback Method
hf	-341.04	kJ/mol	Joback Method
hfus	24.60	kJ/mol	Joback Method
hvap	45.46	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	5.563		Crippen Method
mcvol	208.120	ml/mol	McGowan Method
pc	1546.35	kPa	Joback Method
rinpol	1347.00		NIST Webbook
rinpol	1347.00		NIST Webbook
tb	516.49	K	Joback Method
tc	684.40	K	Joback Method
tf	249.96	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	508.27	J/molxK	516.49	Joback Method
cpg	527.48	J/molxK	544.48	Joback Method
cpg	545.85	J/molxK	572.46	Joback Method
cpg	563.41	J/molxK	600.45	Joback Method
cpg	580.19	J/molxK	628.43	Joback Method
cpg	596.21	J/molxK	656.42	Joback Method
cpg	611.50	J/molxK	684.40	Joback Method
dvisc	0.0082820	Paxs	249.96	Joback Method

dvisc	0.0026796	Paxs	294.38	Joback Method
dvisc	0.0011655	Paxs	338.80	Joback Method
dvisc	0.0006148	Paxs	383.23	Joback Method
dvisc	0.0003704	Paxs	427.65	Joback Method
dvisc	0.0002455	Paxs	472.07	Joback Method
dvisc	0.0001747	Paxs	516.49	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=R415384&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
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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