

Undecane, 5-ethyl-6-methyl

Inchi:	InChI=1S/C14H30/c1-5-8-10-11-13(4)14(7-3)12-9-6-2/h13-14H,5-12H2,1-4H3
InchiKey:	DCYFVLJPOCOBHW-UHFFFAOYSA-N
Formula:	C14H30
SMILES:	CCCCC(C)C(CC)CCCC
Mol. weight [g/mol]:	198.39

Physical Properties

Property code	Value	Unit	Source
gf	62.12	kJ/mol	Joback Method
hf	-342.85	kJ/mol	Joback Method
hfus	24.97	kJ/mol	Joback Method
hvap	45.98	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	5.419		Crippen Method
mcvol	208.120	ml/mol	McGowan Method
pc	1542.71	kPa	Joback Method
rinpol	1288.00		NIST Webbook
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tb	518.84	K	Joback Method
tc	684.31	K	Joback Method
tf	217.54	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.22	J/mol×K	518.84	Joback Method
cpg	525.09	J/mol×K	546.42	Joback Method
cpg	543.22	J/mol×K	574.00	Joback Method
cpg	560.62	J/mol×K	601.58	Joback Method
cpg	577.31	J/mol×K	629.15	Joback Method
cpg	593.31	J/mol×K	656.73	Joback Method
cpg	608.64	J/mol×K	684.31	Joback Method
dvisc	0.0154332	Pa×s	217.54	Joback Method

dvisc	0.0035509	Pa×s	267.76	Joback Method
dvisc	0.0012995	Pa×s	317.97	Joback Method
dvisc	0.0006256	Pa×s	368.19	Joback Method
dvisc	0.0003589	Pa×s	418.41	Joback Method
dvisc	0.0002320	Pa×s	468.62	Joback Method
dvisc	0.0001631	Pa×s	518.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R9995&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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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