

Undecane, 5-butyl-6-propyl

Inchi:	InChI=1S/C18H38/c1-5-9-12-16-17(13-8-4)18(14-10-6-2)15-11-7-3/h17-18H,5-16H2,1-4H
InchiKey:	JDWBYZBVKELQJ-UHFFFAOYSA-N
Formula:	C18H38
SMILES:	CCCCC(CCC)C(CCCC)CCCC
Mol. weight [g/mol]:	254.49

Physical Properties

Property code	Value	Unit	Source
gf	95.80	kJ/mol	Joback Method
hf	-425.41	kJ/mol	Joback Method
hfus	35.33	kJ/mol	Joback Method
hvap	54.89	kJ/mol	Joback Method
log10ws	-6.87		Crippen Method
logp	6.980		Crippen Method
mvol	264.480	ml/mol	McGowan Method
pc	1164.84	kPa	Joback Method
rinpol	1550.00		NIST Webbook
rinpol	1550.00		NIST Webbook
tb	610.36	K	Joback Method
tc	773.50	K	Joback Method
tf	262.62	K	Joback Method
vc	1.032	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.07	J/molxK	610.36	Joback Method
cpg	744.77	J/molxK	637.55	Joback Method
cpg	764.63	J/molxK	664.74	Joback Method
cpg	783.65	J/molxK	691.93	Joback Method
cpg	801.88	J/molxK	719.12	Joback Method
cpg	819.32	J/molxK	746.31	Joback Method
cpg	836.01	J/molxK	773.50	Joback Method
dvisc	0.0097660	Paxs	262.62	Joback Method

dvisc	0.0023312	Paxs	320.58	Joback Method
dvisc	0.0008629	Paxs	378.53	Joback Method
dvisc	0.0004158	Paxs	436.49	Joback Method
dvisc	0.0002378	Paxs	494.45	Joback Method
dvisc	0.0001529	Paxs	552.40	Joback Method
dvisc	0.0001069	Paxs	610.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R9982&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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