Undecane, 5-ethyl-5-propyl-

Other names:	Butyl(ethyl)(hexyl)(propyl)methane
Inchi:	InChI=1S/C16H34/c1-5-9-11-12-15-16(8-4,13-7-3)14-10-6-2/h5-15H2,1-4H3
InchiKey:	MEBZNFSYULDMSV-UHFFFAOYSA-N
Formula:	C16H34
SMILES:	CCCCCCC(CC)(CCC)CCCC
Mol. weight [g/mol]:	226.44
CAS:	2755-07-9

Physical Properties

Property code	Value	Unit	Source
gf	86.68	kJ/mol	Joback Method
hf	-382.32	kJ/mol	Joback Method
hfus	29.78	kJ/mol	Joback Method
hvap	49.91	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	6.344		Crippen Method
mcvol	236.300	ml/mol	McGowan Method
pc	1336.86	kPa	Joback Method
tb	562.25	K	Joback Method
tc	728.23	K	Joback Method
tf	198.00 ± 5.00	K	NIST Webbook
vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.09	J/mol×K	562.25	Joback Method
cpg	634.19	J/mol×K	589.91	Joback Method
cpg	653.40	J/mol×K	617.58	Joback Method
cpg	671.77	J/mol×K	645.24	Joback Method
cpg	689.32	J/mol×K	672.91	Joback Method
cpg	706.10	J/mol×K	700.57	Joback Method
cpg	722.12	J/mol×K	728.23	Joback Method
dvisc	0.0068269	Pa×s	272.50	Joback Method

dvisc	0.0021907	Pa×s	320.79	Joback Method
dvisc	0.0009465	Pa×s	369.08	Joback Method
dvisc	0.0004966	Pa×s	417.38	Joback Method
dvisc	0.0002978	Pa×s	465.67	Joback Method
dvisc	0.0001966	Pa×s	513.96	Joback Method
dvisc	0.0001394	Pa×s	562.25	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2755079&Units=SI

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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