

5-Butyl-5-ethylundecane

Inchi:	InChI=1S/C17H36/c1-5-9-12-13-16-17(8-4,14-10-6-2)15-11-7-3/h5-16H2,1-4H3
InchiKey:	RUEWNCYEYXGUPB-UHFFFAOYSA-N
Formula:	C17H36
SMILES:	CCCCCCC(CC)(CCCC)CCCC
Mol. weight [g/mol]:	240.47

Physical Properties

Property code	Value	Unit	Source
gf	95.10	kJ/mol	Joback Method
hf	-402.96	kJ/mol	Joback Method
hfus	32.37	kJ/mol	Joback Method
hvap	52.14	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	6.734		Crippen Method
mcvol	250.390	ml/mol	McGowan Method
pc	1247.73	kPa	Joback Method
rinpol	1552.00		NIST Webbook
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tb	585.13	K	Joback Method
tc	750.44	K	Joback Method
tf	283.77	K	Joback Method
vc	0.977	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.21	J/molxK	585.13	Joback Method
cpg	762.91	J/molxK	722.89	Joback Method
cpg	745.83	J/molxK	695.34	Joback Method
cpg	727.95	J/molxK	667.79	Joback Method
cpg	709.25	J/molxK	640.23	Joback Method
cpg	689.68	J/molxK	612.68	Joback Method
cpg	779.23	J/molxK	750.44	Joback Method
dvisc	0.0001235	Paxs	585.13	Joback Method

dvisc	0.0001745	Paxs	534.90	Joback Method
dvisc	0.0002647	Paxs	484.68	Joback Method
dvisc	0.0004422	Paxs	434.45	Joback Method
dvisc	0.0008449	Paxs	384.22	Joback Method
dvisc	0.0019614	Paxs	334.00	Joback Method
dvisc	0.0061345	Paxs	283.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R415611&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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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