Undecane, 6-butyl

Inchi: InChI=1S/C15H32/c1-4-7-10-13-15(12-9-6-3)14-11-8-5-2/h15H,4-14H2,1-3H3
InchiKey: WLSWCYRKJDHEIN-UHFFFAOYSA-N
Formula: C15H32
SMILES: CCCCCC(CCCC)CCCCC
Mol. weight [g/mol]: 212.41

Physical Properties

Property code	Value	Unit	Source
gf	72.98	kJ/mol	Joback Method
hf	-358.21	kJ/mol	Joback Method
hfus	31.08	kJ/mol	Joback Method
hvap	48.60	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.953		Crippen Method
mcvol	222.210	ml/mol	McGowan Method
pc	1423.99	kPa	Joback Method
rinpol	1388.00		NIST Webbook
tb	542.16	K	Joback Method
tc	703.93	K	Joback Method
tf	243.81	K	Joback Method
vc	0.870	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.22	J/mol×K	542.16	Joback Method
cpg	577.24	J/mol×K	569.12	Joback Method
cpg	595.52	J/mol×K	596.08	Joback Method
cpg	613.07	J/mol×K	623.04	Joback Method
cpg	629.92	J/mol×K	650.00	Joback Method
cpg	646.08	J/mol×K	676.97	Joback Method
cpg	661.59	J/mol×K	703.93	Joback Method
dvisc	0.0083877	Pa×s	243.81	Joback Method
dvisc	0.0024681	Pa×s	293.53	Joback Method

dvisc	0.0010352	Pa×s	343.26	Joback Method
dvisc	0.0005409	Pa×s	392.99	Joback Method
dvisc	0.0003270	Pa×s	442.71	Joback Method
dvisc	0.0002189	Pa×s	492.43	Joback Method
dvisc	0.0001577	Pa×s	542.16	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=R10016&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