Cyclohexane, 1-propylbutyl

Inchi: InChI=1S/C13H26/c1-3-8-12(9-4-2)13-10-6-5-7-11-13/h12-13H,3-11H2,1-2H3
InchiKey: LMTXDXIKTNVOAL-UHFFFAOYSA-N
Formula: C13H26
SMILES: CCCC(CCC)C1CCCCC1
Mol. weight [g/mol]: 182.35

Physical Properties

Property code	Value	Unit	Source
gf	80.59	kJ/mol	Joback Method
hf	-262.61	kJ/mol	Joback Method
hfus	17.74	kJ/mol	Joback Method
hvap	44.57	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.783		Crippen Method
mcvol	183.170	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1321.00		NIST Webbook
rinpol	1321.00		NIST Webbook
tb	515.95	K	Joback Method
tc	709.95	K	Joback Method
tf	228.65	K	Joback Method
vc	0.691	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.63	J/mol×K	515.95	Joback Method
cpg	467.60	J/mol×K	548.28	Joback Method
cpg	488.49	J/mol×K	580.62	Joback Method
cpg	508.34	J/mol×K	612.95	Joback Method
cpg	527.16	J/mol×K	645.28	Joback Method
cpg	545.00	J/mol×K	677.61	Joback Method
cpg	561.88	J/mol×K	709.95	Joback Method
dvisc	0.0127535	Pa×s	228.65	Joback Method

dvisc	0.0035288	Pa×s	276.53	Joback Method
dvisc	0.0014268	Pa×s	324.42	Joback Method
dvisc	0.0007282	Pa×s	372.30	Joback Method
dvisc	0.0004332	Pa×s	420.18	Joback Method
dvisc	0.0002866	Pa×s	468.07	Joback Method
dvisc	0.0002047	Pa×s	515.95	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=R133329&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