Cyclohexene,3-hexyl-

Other names: 3-hexyl-1-cyclohexene
Inchi: InChI=1S/C12H22/c1-2-3-4-6-9-12-10-7-5-8-11-12/h7,10,12H,2-6,8-9,11H2,1H3
InchiKey: OQKLIIQHYMWPMF-UHFFFAOYSA-N
Formula: C12H22
SMILES: CCCCCCC1C=CCCC1
Mol. weight [g/mol]: 166.30
CAS: 15232-78-7

Physical Properties

Property code	Value	Unit	Source
gf	104.57	kJ/mol	Joback Method
hf	-178.91	kJ/mol	Joback Method
hfus	19.89	kJ/mol	Joback Method
hvap	43.03	kJ/mol	Joback Method
ie	8.78 ± 0.01	eV	NIST Webbook
log10ws	-4.35		Crippen Method
logp	4.313		Crippen Method
mcvol	164.780	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	1243.00		NIST Webbook
ripol	1398.00		NIST Webbook
ripol	1406.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1423.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1401.00		NIST Webbook
ripol	1403.00		NIST Webbook
ripol	1409.00		NIST Webbook
ripol	1375.20		NIST Webbook
ripol	1381.00		NIST Webbook
ripol	1386.70		NIST Webbook
ripol	1392.30		NIST Webbook
ripol	1397.90		NIST Webbook
ripol	1402.80		NIST Webbook

ripol	1409.20		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1355.70		NIST Webbook
ripol	1352.00		NIST Webbook
ripol	1344.30		NIST Webbook
tb	492.67	K	Joback Method
tc	686.75	K	Joback Method
tf	233.14	K	Joback Method
vc	0.626	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	378.39	J/mol×K	492.67	Joback Method
cpg	398.23	J/mol×K	525.02	Joback Method
cpg	417.08	J/mol×K	557.36	Joback Method
cpg	434.99	J/mol×K	589.71	Joback Method
cpg	451.98	J/mol×K	622.06	Joback Method
cpg	468.07	J/mol×K	654.40	Joback Method
cpg	483.31	J/mol×K	686.75	Joback Method
dvisc	0.0064172	Pa×s	233.14	Joback Method
dvisc	0.0023940	Pa×s	276.39	Joback Method
dvisc	0.0011663	Pa×s	319.65	Joback Method
dvisc	0.0006744	Pa×s	362.90	Joback Method
dvisc	0.0004383	Pa×s	406.16	Joback Method
dvisc	0.0003094	Pa×s	449.41	Joback Method
dvisc	0.0002322	Pa×s	492.67	Joback Method

Sources

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=C15232787&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume