1-Heptylcyclohexene

Other names: Cyclohexene,1-heptyl-
1-Heptyl-1-cyclohexene
Inchi: InChI=1S/C13H24/c1-2-3-4-5-7-10-13-11-8-6-9-12-13/h11H,2-10,12H2,1H3
InchiKey: XDUFGMTUKHRHSO-UHFFFAOYSA-N
Formula: C13H24
SMILES: CCCCCCCC1=CCCCC1
Mol. weight [g/mol]: 180.33
CAS: 15232-86-7

Physical Properties

Property code	Value	Unit	Source
gf	111.07	kJ/mol	Joback Method
hf	-190.68	kJ/mol	Joback Method
hfus	21.02	kJ/mol	Joback Method
hvap	46.22	kJ/mol	Joback Method
ie	8.37 ± 0.02	eV	NIST Webbook
log10ws	-5.01		Crippen Method
logp	4.847		Crippen Method
mcvol	178.870	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1344.00		NIST Webbook
rinpol	1342.00		NIST Webbook
ripol	1499.10		NIST Webbook
ripol	1504.00		NIST Webbook
ripol	1476.80		NIST Webbook
ripol	1482.50		NIST Webbook
ripol	1488.20		NIST Webbook
ripol	1493.40		NIST Webbook
ripol	1499.00		NIST Webbook
ripol	1503.90		NIST Webbook
ripol	1486.00		NIST Webbook
ripol	1493.00		NIST Webbook
ripol	1488.00		NIST Webbook
ripol	1482.00		NIST Webbook
ripol	1477.00		NIST Webbook
ripol	1470.00		NIST Webbook
ripol	1518.00		NIST Webbook

ripol	1513.00		NIST Webbook
ripol	1501.00		NIST Webbook
ripol	1498.00		NIST Webbook
ripol	1486.00		NIST Webbook
tb	525.20	K	Joback Method
tc	718.22	K	Joback Method
tf	261.17	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.76	J/mol×K	525.20	Joback Method
cpg	517.75	J/mol×K	686.05	Joback Method
cpg	501.78	J/mol×K	653.88	Joback Method
cpg	484.92	J/mol×K	621.71	Joback Method
cpg	467.15	J/mol×K	589.54	Joback Method
cpg	448.44	J/mol×K	557.37	Joback Method
cpg	532.88	J/mol×K	718.22	Joback Method
dvisc	0.0001931	Pa×s	525.20	Joback Method
dvisc	0.0002624	Pa×s	481.20	Joback Method
dvisc	0.0003791	Pa×s	437.19	Joback Method
dvisc	0.0005948	Pa×s	393.19	Joback Method
dvisc	0.0010454	Pa×s	349.18	Joback Method
dvisc	0.0021619	Pa×s	305.18	Joback Method
dvisc	0.0057111	Pa×s	261.17	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15232867&Units=SI

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

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