

Benzene, (1-cyclohexylethyl)-

Other names:

Ethane, 1-cyclohexyl-1-phenyl-
(«alpha»-Methylbenzyl)cyclohexane
1-Phenyl-1-cyclohexylethane
1-Cyclohexyl-1-phenylethane

Inchi:

InChI=1S/C14H20/c1-12(13-8-4-2-5-9-13)14-10-6-3-7-11-14/h2,4-5,8-9,12,14H,3,6-7,10-

InchiKey:

HNBZJZFPJDFJMLP-UHFFFAOYSA-N

Formula:

C14H20

SMILES:

CC(c1cccc1)C1CCCCC1

Mol. weight [g/mol]:

188.31

CAS:

4413-16-5

Physical Properties

Property code	Value	Unit	Source
gf	201.42	kJ/mol	Joback Method
hf	-46.72	kJ/mol	Joback Method
hfus	14.37	kJ/mol	Joback Method
hvap	49.08	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.370		Crippen Method
mcvol	173.500	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
tb	565.51	K	Joback Method
tc	802.24	K	Joback Method
tf	219.26 ± 0.27	K	NIST Webbook
vc	0.638	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.39	J/molxK	802.24	Joback Method
cpg	432.53	J/molxK	565.51	Joback Method
cpg	455.40	J/molxK	604.96	Joback Method
cpg	476.68	J/molxK	644.42	Joback Method
cpg	496.45	J/molxK	683.87	Joback Method

cpg	514.78	J/mol×K	723.33	Joback Method
cpg	531.74	J/mol×K	762.78	Joback Method
dvisc	0.0001828	Paxs	565.51	Joback Method
dvisc	0.0068481	Paxs	266.34	Joback Method
dvisc	0.0023255	Paxs	316.20	Joback Method
dvisc	0.0010599	Paxs	366.06	Joback Method
dvisc	0.0005832	Paxs	415.93	Joback Method
dvisc	0.0003647	Paxs	465.79	Joback Method
dvisc	0.0002497	Paxs	515.65	Joback Method
hvapt	70.80	kJ/mol	379.50	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C4413165&Units=SI

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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