Benzene, hexaethyl-

Other names: HEXAETENZEE
Hexaethylbenzene
Inchi: InChI=1S/C18H30/c1-7-13-14(8-2)16(10-4)18(12-6)17(11-5)15(13)9-3/h7-12H2,1-6H3
InchiKey: LXSMILGNHYBUCG-UHFFFAOYSA-N
Formula: C18H30
SMILES: CCc1c(CC)c(CC)c(CC)c(CC)c1CC
Mol. weight [g/mol]: 246.43
CAS: 604-88-6

Physical Properties

Property code	Value	Unit	Source
af	0.6980		KDB
chs	-11026.60 ± 5.60	kJ/mol	NIST Webbook
gf	164.94	kJ/mol	Joback Method
hf	-235.67	kJ/mol	Joback Method
hfus	34.47	kJ/mol	Joback Method
hsub	41.30 ± 0.92	kJ/mol	NIST Webbook
hvap	61.25	kJ/mol	Joback Method
ie	7.71	eV	NIST Webbook
log10ws	-6.29		Crippen Method
logp	5.061		Crippen Method
mcvol	240.720	ml/mol	McGowan Method
pc	1380.00	kPa	KDB
rinpol	1706.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1699.00		NIST Webbook
rinpol	1658.00		NIST Webbook
rinpol	1689.00		NIST Webbook
rinpol	1682.00		NIST Webbook
rinpol	1682.00		NIST Webbook
tb	571.20	K	KDB
tb	571.20	K	NIST Webbook
tc	734.80	K	KDB
tf	400.00 ± 2.00	K	NIST Webbook
tf	401.65 ± 1.00	K	NIST Webbook
tf	401.00	K	KDB
tf	402.30 ± 1.00	K	NIST Webbook

vc	0.935	m3/kmol	KDB
zc	0.2113090		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.73	J/mol×K	821.05	Joback Method
cpg	725.19	J/mol×K	789.40	Joback Method
cpg	708.85	J/mol×K	757.76	Joback Method
cpg	691.68	J/mol×K	726.11	Joback Method
cpg	673.65	J/mol×K	694.47	Joback Method
cpg	654.76	J/mol×K	662.82	Joback Method
cpg	755.46	J/mol×K	852.69	Joback Method
dvisc	0.0008584	Pa×s	381.64	Joback Method
dvisc	0.0001184	Pa×s	662.82	Joback Method
dvisc	0.0001452	Pa×s	615.96	Joback Method
dvisc	0.0001843	Pa×s	569.09	Joback Method
dvisc	0.0002441	Pa×s	522.23	Joback Method
dvisc	0.0003418	Pa×s	475.37	Joback Method
dvisc	0.0005151	Pa×s	428.50	Joback Method
hsubt	95.00 ± 4.00	kJ/mol	339.50	NIST Webbook
hvapt	62.60	kJ/mol	489.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55137e+01
Coeff. B	-5.65320e+03
Coeff. C	-5.23390e+01
Temperature range (K), min.	423.15
Temperature range (K), max.	606.15

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2

Coeff. A	7.60815e+01
Coeff. B	-1.05315e+04
Coeff. C	-8.50968e+00
Coeff. D	3.03545e-06
Temperature range (K), min.	427.00
Temperature range (K), max.	591.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C604886&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=715
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol715.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
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
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility