Pentaethylbenzene

Other names: 1-PENTAETHYLBENZENE
Benzene, pentaethyl-
Inchi: InChI=1S/C16H26/c1-6-12-11-13(7-2)15(9-4)16(10-5)14(12)8-3/h11H,6-10H2,1-5H3
InchiKey: JREJWHNDQOGSQT-UHFFFAOYSA-N
Formula: C16H26
SMILES: CCc1cc(CC)c(CC)c(CC)c1CC
Mol. weight [g/mol]: 218.38
CAS: 605-01-6

Physical Properties

Property code	Value	Unit	Source
gf	157.73	kJ/mol	Joback Method
hf	-182.92	kJ/mol	Joback Method
hfus	29.68	kJ/mol	Joback Method
hvap	56.13	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.499		Crippen Method
mcvol	212.540	ml/mol	McGowan Method
pc	1621.98	kPa	Joback Method
rinpol	1538.00		NIST Webbook
tb	612.08	K	Joback Method
tc	805.10	K	Joback Method
tf	346.58	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.12	J/mol×K	612.08	Joback Method
cpg	564.31	J/mol×K	644.25	Joback Method
cpg	581.66	J/mol×K	676.42	Joback Method
cpg	598.19	J/mol×K	708.59	Joback Method
cpg	613.93	J/mol×K	740.76	Joback Method
cpg	628.88	J/mol×K	772.93	Joback Method

cpg	643.08	J/mol×K	805.10	Joback Method
dvisc	0.0011135	Pa×s	346.58	Joback Method
dvisc	0.0006505	Pa×s	390.83	Joback Method
dvisc	0.0004239	Pa×s	435.08	Joback Method
dvisc	0.0002990	Pa×s	479.33	Joback Method
dvisc	0.0002237	Pa×s	523.58	Joback Method
dvisc	0.0001751	Pa×s	567.83	Joback Method
dvisc	0.0001420	Pa×s	612.08	Joback Method
hvapt	56.50	kJ/mol	454.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	-5.97616e+00
Coeff. B	-5.95488e+03
Coeff. C	3.56766e+00
Coeff. D	-3.68029e-06
Temperature range (K), min.	359.15
Temperature range (K), max.	723.64

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C605016&Units=SI
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=713
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/mol713.mol

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume