benzene, 1,2,3,5-tetraethyl-

Other names:	1,2,3,5-Tetraethylbenzene
Inchi:	InChI=1S/C14H22/c1-5-11-9-12(6-2)14(8-4)13(7-3)10-11/h9-10H,5-8H2,1-4H3
InchiKey:	QJEXLOSCNXHBAX-UHFFFAOYSA-N
Formula:	C14H22
SMILES:	CCc1cc(CC)c(CC)c(CC)c1
Mol. weight [g/mol]:	190.32
CAS:	38842-05-6

Physical Properties

Property code	Value	Unit	Source
gf	150.52	kJ/mol	Joback Method
hf	-130.17	kJ/mol	Joback Method
hfus	24.89	kJ/mol	Joback Method
hvap	51.02	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.936		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	1390.00		NIST Webbook
tb	561.34	K	Joback Method
tc	758.43	K	Joback Method
tf	252.00 ± 2.00	K	NIST Webbook
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.27	J/mol×K	561.34	Joback Method
cpg	460.57	J/mol×K	594.19	Joback Method
cpg	477.05	J/mol×K	627.04	Joback Method
cpg	492.74	J/mol×K	659.89	Joback Method
cpg	507.66	J/mol×K	692.73	Joback Method
cpg	521.83	J/mol×K	725.58	Joback Method
cpg	535.27	J/mol×K	758.43	Joback Method

dvisc	0.0014453	Pa×s	311.52	Joback Method
dvisc	0.0008167	Pa×s	353.16	Joback Method
dvisc	0.0005205	Pa×s	394.79	Joback Method
dvisc	0.0003615	Pa×s	436.43	Joback Method
dvisc	0.0002676	Pa×s	478.07	Joback Method
dvisc	0.0002078	Pa×s	519.70	Joback Method
dvisc	0.0001675	Pa×s	561.34	Joback Method
hvapt	64.80	kJ/mol	467.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42717e+01
Coeff. B	-4.62805e+03
Coeff. C	-5.45830e+01
Temperature range (K), min.	385.53
Temperature range (K), max.	571.09

Sources

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/mol709.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38842056&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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