BENZENE, 1,2,4,5-TETRAETHYL-

Other names: 1,2,4,5-Tetraethylbenzene
Inchi: InChI=1S/C14H22/c1-5-11-9-13(7-3)14(8-4)10-12(11)6-2/h9-10H,5-8H2,1-4H3
InchiKey: NSOYZSQQDPNCAC-UHFFFAOYSA-N
Formula: C14H22
SMILES: CCc1cc(CC)c(CC)cc1CC
Mol. weight [g/mol]: 190.33
CAS: 635-81-4

Physical Properties

Property code	Value	Unit	Source
af	0.5597		Cheméo Relay (1.0)
gf	150.52	kJ/mol	Joback Method
hf	-106.08	kJ/mol	Cheméo Relay (1.0)
hfus	24.89	kJ/mol	Joback Method
hvap	68.99	kJ/mol	Cheméo Relay (1.0)
ie	8.01	eV	Cheméo Relay (1.0)
log10ws	-5.63		Cheméo Relay (1.0)
logp	3.936		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	1388.00		NIST Webbook
tb	522.16	K	Cheméo Relay (1.0)
tc	710.41	K	Cheméo Relay (1.0)
tf	283.00 ± 2.00	K	NIST Webbook
tf	283.00 ± 2.00	K	NIST Webbook
vc	0.705	m3/kmol	Cheméo Relay (1.0)

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	54.50	kJ/mol	429.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42990e+01
Coeff. B	-4.63058e+03
Coeff. C	-5.56700e+01
Temperature range (K), min.	386.16
Temperature range (K), max.	570.90

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C635814&Units=SI

Cheméo Relay (1.0, beta):

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Cheméo Relay (1.0):

KDB: https://www.cheric.org/files/research/kdb/mol/mol710.mol

Legend

af:	Acentric Factor
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
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