Benzene, 1-ethyl-4-(phenylmethyl)-

Other names:	1-Ethyl-4-benzylbenzene
	4'-Ethyldiphenylmethane
	4-Ethyldiphenylmethane
	Methane, (p-ethylphenyl)phenyl-
Inchi:	InChI=1S/C15H16/c1-2-13-8-10-15(11-9-13)12-14-6-4-3-5-7-14/h3-11H,2,12H2,1H3
InchiKey:	HSHDPVRGPKOGME-UHFFFAOYSA-N
Formula:	C15H16
SMILES:	CCc1ccc(Cc2ccccc2)cc1
Mol. weight [g/mol]:	196.29
CAS:	620-85-9

Physical Properties

Property code	Value	Unit	Source
af	0.4846		Cheméo Relay (1.0)
chl	-8196.00	kJ/mol	NIST Webbook
gf	290.61	kJ/mol	Joback Method
hf	128.83	kJ/mol	Cheméo Relay (1.0)
hfus	22.30	kJ/mol	Joback Method
hvap	77.15	kJ/mol	Cheméo Relay (1.0)
ie	8.54	eV	Cheméo Relay (1.0)
log10ws	-5.13		Cheméo Relay (1.0)
logp	3.840		Crippen Method
mcvol	174.690	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinpol	278.60		NIST Webbook
tb	570.18 ± 0.30	K	NIST Webbook
tb	570.18 ± 0.30	K	NIST Webbook
tc	785.80	K	Cheméo Relay (1.0)
tf	249.63 ± 0.20	K	NIST Webbook
tf	249.63 ± 0.20	K	NIST Webbook
vc	0.664	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.35	J/mol×K	600.94	Joback Method
cpg	439.33	J/mol×K	640.22	Joback Method
cpg	456.02	J/mol×K	679.51	Joback Method
cpg	471.49	J/mol×K	718.79	Joback Method
cpg	485.83	J/mol×K	758.08	Joback Method
cpg	499.09	J/mol×K	797.36	Joback Method
cpg	511.34	J/mol×K	836.65	Joback Method
dvisc	0.0019137	Pa×s	324.17	Joback Method
dvisc	0.0009812	Pa×s	370.30	Joback Method
dvisc	0.0005833	Pa×s	416.43	Joback Method
dvisc	0.0003847	Pa×s	462.56	Joback Method
dvisc	0.0002736	Pa×s	508.68	Joback Method
dvisc	0.0002059	Pa×s	554.81	Joback Method
dvisc	0.0001619	Pa×s	600.94	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46642e+01
Coeff. B	-4.81793e+03
Coeff. C	-9.05850e+01
Temperature range (K), min.	425.71
Temperature range (K), max.	605.72

Sources

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C620859&Units=SI

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

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

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

Legend

af:	Acentric Factor
chl:	Standard liquid 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
hvap:	Enthalpy of vaporization at standard conditions
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