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

Other names: 1-Ethyl-4-isopropylbenzene
Cumene, p-ethyl-
Inchi: InChI=1S/C11H16/c1-4-10-5-7-11(8-6-10)9(2)3/h5-9H,4H2,1-3H3
InchiKey: GUUDUUDWUWUTPD-UHFFFAOYSA-N
Formula: C11H16
SMILES: CCc1ccc(C(C)C)cc1
Mol. weight [g/mol]: 148.24
CAS: 4218-48-8

Physical Properties

Property code	Value	Unit	Source
gf	142.08	kJ/mol	Joback Method
hf	-50.59	kJ/mol	Joback Method
hfus	14.37	kJ/mol	Joback Method
hvap	42.63	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.372		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
rinpol	1094.50		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1103.00		NIST Webbook
rinpol	1111.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1114.30		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1104.00		NIST Webbook
rinpol	1102.45		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1104.90		NIST Webbook

rinpol	1105.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1114.00		NIST Webbook
rinpol	1094.50		NIST Webbook
rinpol	1097.30		NIST Webbook
rinpol	1097.30		NIST Webbook
rinpol	1110.10		NIST Webbook
rinpol	1114.30		NIST Webbook
rinpol	1102.45		NIST Webbook
ripol	1323.30		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1362.00		NIST Webbook
ripol	1374.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1398.00		NIST Webbook
ripol	1323.00		NIST Webbook
ripol	1350.00		NIST Webbook
tb	471.00 ± 4.00	K	NIST Webbook
tb	471.00 ± 4.00	K	NIST Webbook
tb	471.00 ± 6.00	K	NIST Webbook
tb	471.00 ± 6.00	K	NIST Webbook
tc	690.17	K	Joback Method
tf	253.15 ± 5.00	K	NIST Webbook
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.93	J/mol×K	482.30	Joback Method
cpg	317.03	J/mol×K	516.94	Joback Method
cpg	332.27	J/mol×K	551.59	Joback Method
cpg	346.68	J/mol×K	586.23	Joback Method
cpg	360.30	J/mol×K	620.88	Joback Method
cpg	373.16	J/mol×K	655.52	Joback Method
cpg	385.28	J/mol×K	690.17	Joback Method
dvisc	0.0036688	Pa×s	237.67	Joback Method
dvisc	0.0015812	Pa×s	278.44	Joback Method
dvisc	0.0008449	Pa×s	319.21	Joback Method
dvisc	0.0005204	Pa×s	359.99	Joback Method
dvisc	0.0003537	Pa×s	400.76	Joback Method
dvisc	0.0002582	Pa×s	441.53	Joback Method

dvisc	0.0001987	Pa×s	482.30	Joback Method
hvapt	49.40	kJ/mol	386.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42800e+01
Coeff. B	-3.84773e+03
Coeff. C	-7.15040e+01
Temperature range (K), min.	346.49
Temperature range (K), max.	500.53

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4218488&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume