Benzene, 1-bromo-4-ethyl-

Other names:	1-Bromo-4-ethylbenzene
	4-Ethylbromobenzene
	p-Bromoethylbenzene
	p-Ethylbromobenzene
Inchi:	InChI=1S/C8H9Br/c1-2-7-3-5-8(9)6-4-7/h3-6H,2H2,1H3
InchiKey:	URFPRAHGGBYNPW-UHFFFAOYSA-N
Formula:	C8H9Br
SMILES:	CCc1ccc(Br)cc1
Mol. weight [g/mol]:	185.06
CAS:	1585-07-5

Physical Properties

Property code	Value	Unit	Source
gf	133.58	kJ/mol	Joback Method
hf	42.94	kJ/mol	Joback Method
hfus	15.41	kJ/mol	Joback Method
hvap	42.78	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	3.012		Crippen Method
mcvol	117.320	ml/mol	McGowan Method
pc	3901.37	kPa	Joback Method
tb	478.22 ± 0.07	K	NIST Webbook
tb	477.20	K	NIST Webbook
tc	710.10	K	Joback Method
tf	229.68 ± 0.05	K	NIST Webbook
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	255.40	J/mol×K	633.48	Joback Method
cpg	272.56	J/mol×K	710.10	Joback Method
cpg	264.29	J/mol×K	671.79	Joback Method
cpg	212.97	J/mol×K	480.26	Joback Method

cpg	224.69	J/mol×K	518.57	Joback Method
cpg	235.65	J/mol×K	556.87	Joback Method
cpg	245.87	J/mol×K	595.18	Joback Method
dvisc	0.0002886	Pa×s	480.26	Joback Method
dvisc	0.0004529	Pa×s	413.06	Joback Method
dvisc	0.0003554	Pa×s	446.66	Joback Method
dvisc	0.0021418	Pa×s	278.66	Joback Method
dvisc	0.0012813	Pa×s	312.26	Joback Method
dvisc	0.0008469	Pa×s	345.86	Joback Method
dvisc	0.0006024	Pa×s	379.46	Joback Method
hvapt	52.00	kJ/mol	391.00	NIST Webbook
hvapt	49.40	kJ/mol	455.50	NIST Webbook
hvapt	46.20	kJ/mol	413.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41003e+01
Coeff. B	-3.82504e+03
Coeff. C	-7.37980e+01
Temperature range (K), min.	350.72
Temperature range (K), max.	509.02

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1585075&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume