Benzene, 2-bromo-1,4-dimethyl-

Other names:	1-Bromo-2,5-dimethylbenzene
	2,5-Dimethylbromobenzene
	2,5-Dimethylphenyl bromide
	2,5-Xylyl bromide
	2-Bromo-1,4-dimethylbenzene
	2-Bromo-1,4-xylene
	2-Bromo-p-xylene
	Bromo-p-xylene
	NSC 8051
	p-Xylene, 2-bromo-
Inchi:	InChI=1S/C8H9Br/c1-6-3-4-7(2)8(9)5-6/h3-5H,1-2H3
InchiKey:	QXISTPDUYKNPLU-UHFFFAOYSA-N
Formula:	C8H9Br
SMILES:	Cc1ccc(C)c(Br)c1
Mol. weight [g/mol]:	185.06
CAS:	553-94-6

Physical Properties

Property code	Value	Unit	Source
gf	123.95	kJ/mol	Joback Method
hf	31.47	kJ/mol	Joback Method
hfus	15.02	kJ/mol	Joback Method
hvap	43.44	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.066		Crippen Method
mcvol	117.320	ml/mol	McGowan Method
pc	3829.28	kPa	Joback Method
rinpol	1126.70		NIST Webbook
tb	471.50 ± 0.50	K	NIST Webbook
tb	472.70	K	NIST Webbook
tc	716.43	K	Joback Method
tf	282.00	K	NIST Webbook
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	262.68	J/mol×K	677.90	Joback Method
cpg	253.98	J/mol×K	639.37	Joback Method
cpg	244.68	J/mol×K	600.83	Joback Method
cpg	234.76	J/mol×K	562.30	Joback Method
cpg	224.18	J/mol×K	523.77	Joback Method
cpg	212.91	J/mol×K	485.24	Joback Method
cpg	270.81	J/mol×K	716.43	Joback Method
dvisc	0.0016069	Pa×s	291.18	Joback Method
dvisc	0.0002772	Pa×s	485.24	Joback Method
dvisc	0.0003347	Pa×s	452.90	Joback Method
dvisc	0.0004159	Pa×s	420.55	Joback Method
dvisc	0.0005358	Pa×s	388.21	Joback Method
dvisc	0.0007230	Pa×s	355.87	Joback Method
dvisc	0.0010357	Pa×s	323.52	Joback Method
hvapt	50.90	kJ/mol	395.00	NIST Webbook
hvapt	53.60	kJ/mol	395.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	376.50 ± 1.50	K	3.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40482e+01
Coeff. B	-3.77470e+03
Coeff. C	-7.24080e+01
Temperature range (K), min.	346.72
Temperature range (K), max.	504.46

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=C553946&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume