

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

Other names:	1,3-Dimethyl-4-bromobenzene 1-Bromo-2,4-dimethylbenzene 2,4-Dimethylbromobenzene 4-Bromo-m-xylene m-Xylene, 4-bromo-
Inchi:	InChI=1S/C8H9Br/c1-6-3-4-8(9)7(2)5-6/h3-5H,1-2H3
InchiKey:	YSFLQVNTBBUKEA-UHFFFAOYSA-N
Formula:	C8H9Br
SMILES:	Cc1ccc(Br)c(C)c1
Mol. weight [g/mol]:	185.06
CAS:	583-70-0

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
tb	478.00	K	NIST Webbook
tb	487.20	K	NIST Webbook
tb	478.20	K	NIST Webbook
tc	716.43	K	Joback Method
tf	291.18	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.91	J/molxK	485.24	Joback Method
cpg	262.68	J/molxK	677.90	Joback Method

cpg	253.98	J/molxK	639.37	Joback Method
cpg	244.68	J/molxK	600.83	Joback Method
cpg	234.76	J/molxK	562.30	Joback Method
cpg	224.18	J/molxK	523.77	Joback Method
cpg	270.81	J/molxK	716.43	Joback Method
dvisc	0.0002772	Paxs	485.24	Joback Method
dvisc	0.0003347	Paxs	452.90	Joback Method
dvisc	0.0004159	Paxs	420.55	Joback Method
dvisc	0.0005358	Paxs	388.21	Joback Method
dvisc	0.0007230	Paxs	355.87	Joback Method
dvisc	0.0010357	Paxs	323.52	Joback Method
dvisc	0.0016069	Paxs	291.18	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.34740e+01
Coeff. B	-3.65849e+03
Coeff. C	-7.40760e+01
Temperature range (K), min.	351.52
Temperature range (K), max.	522.28

Sources

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=C583700&Units=SI
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/ci9903071

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
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

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