

Benzene, 1-bromo-3,5-dimethyl-

Other names:	m-Xylene, 5-bromo- 3,5-Dimethylbromobenzene 5-Bromo-m-xylene 5-Bromo-1,3-xylene
Inchi:	InChI=1S/C8H9Br/c1-6-3-7(2)5-8(9)4-6/h3-5H,1-2H3
InchiKey:	LMFRTSBQRLSJHC-UHFFFAOYSA-N
Formula:	C8H9Br
SMILES:	Cc1cc(C)cc(Br)c1
Mol. weight [g/mol]:	185.06
CAS:	556-96-7

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 ± 1.00	K	NIST Webbook
tb	477.20	K	NIST Webbook
tc	716.43	K	Joback Method
tf	291.18	K	Joback Method
vc	0.438	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.91	J/mol×K	485.24	Joback Method
cpg	224.18	J/mol×K	523.77	Joback Method
cpg	234.76	J/mol×K	562.30	Joback Method
cpg	244.68	J/mol×K	600.83	Joback Method

cpg	253.98	J/molxK	639.37	Joback Method
cpg	262.68	J/molxK	677.90	Joback Method
cpg	270.81	J/molxK	716.43	Joback Method
dvisc	0.0016069	Paxs	291.18	Joback Method
dvisc	0.0010357	Paxs	323.52	Joback Method
dvisc	0.0007230	Paxs	355.87	Joback Method
dvisc	0.0005358	Paxs	388.21	Joback Method
dvisc	0.0004159	Paxs	420.55	Joback Method
dvisc	0.0003347	Paxs	452.90	Joback Method
dvisc	0.0002772	Paxs	485.24	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.50 ± 0.50	K	1.60	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C556967&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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