Benzene, 2-bromo-1,3,5-trimethyl-

Other names:	1-Bromo-2,4,6-trimethylbenzene
	2,4,6-Trimethylbromobenzene
	2,4,6-Trimethylphenyl bromide
	2-Bromo-1,3,5-trimethylbenzene
	2-Bromomesitylene
	Bromomesitylene
	Mesityl bromide
	Mesitylene, 2-bromo-
	NSC 8064
Inchi:	InChI=1S/C9H11Br/c1-6-4-7(2)9(10)8(3)5-6/h4-5H,1-3H3
InchiKey:	RRTLQRYOJOSPEA-UHFFFAOYSA-N
Formula:	C9H11Br
SMILES:	Cc1cc(C)c(Br)c(C)c1
Mol. weight [g/mol]:	199.09
CAS:	576-83-0

Physical Properties

Property code	Value	Unit	Source
gf	122.74	kJ/mol	Joback Method
hf	-0.64	kJ/mol	Joback Method
hfus	17.23	kJ/mol	Joback Method
hvap	46.33	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.374		Crippen Method
mcvol	131.410	ml/mol	McGowan Method
pc	3352.86	kPa	Joback Method
rinpol	1254.00		NIST Webbook
rinpol	1239.50		NIST Webbook
tb	498.00	K	NIST Webbook
tb	498.20	K	NIST Webbook
tc	741.49	K	Joback Method
tf	314.97	K	Joback Method
vc	0.493	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.32	J/mol×K	513.10	Joback Method
cpg	308.23	J/mol×K	703.42	Joback Method
cpg	298.70	J/mol×K	665.36	Joback Method
cpg	288.57	J/mol×K	627.29	Joback Method
cpg	277.81	J/mol×K	589.23	Joback Method
cpg	266.40	J/mol×K	551.16	Joback Method
cpg	317.20	J/mol×K	741.49	Joback Method
dvisc	0.0002530	Pa×s	513.10	Joback Method
dvisc	0.0003021	Pa×s	480.08	Joback Method
dvisc	0.0003702	Pa×s	447.06	Joback Method
dvisc	0.0004687	Pa×s	414.04	Joback Method
dvisc	0.0006182	Pa×s	381.01	Joback Method
dvisc	0.0008593	Pa×s	347.99	Joback Method
dvisc	0.0012798	Pa×s	314.97	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.20	K	2.10	NIST Webbook
tbrp	382.00 ± 1.00	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41588e+01
Coeff. B	-3.99330e+03
Coeff. C	-7.96360e+01
Temperature range (K), min.	367.52
Temperature range (K), max.	530.99

Sources

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=C576830&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/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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