Benzene, 3-bromo-1,2,4,5-tetramethyl-

Other names:	1-Bromo-2,3,5,6-tetramethylbenzene
	2,3,5,6-Tetramethylbromobenzene
	3-Bromo-1,2,4,5-tetramethylbenzene
	3-Bromodurene
	Bromodurene
	Duryl bromide
Inchi:	InChI=1S/C10H13Br/c1-6-5-7(2)9(4)10(11)8(6)3/h5H,1-4H3
InchiKey:	WJKBPTLQJXKEHC-UHFFFAOYSA-N
Formula:	C10H13Br
SMILES:	Cc1cc(C)c(C)c(Br)c1C
Mol. weight [g/mol]:	213.11
CAS:	1646-53-3

Physical Properties

Property code	Value	Unit	Source
gf	121.53	kJ/mol	Joback Method
hf	-32.75	kJ/mol	Joback Method
hfus	19.43	kJ/mol	Joback Method
hvap	49.21	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.683		Crippen Method
mcvol	145.500	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
tb	540.96	K	Joback Method
tc	766.39	K	Joback Method
tf	338.76	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.48	J/mol×K	540.96	Joback Method
cpg	310.32	J/mol×K	578.53	Joback Method
cpg	322.50	J/mol×K	616.10	Joback Method

cpg	334.03	J/mol×K	653.68	Joback Method
cpg	344.94	J/mol×K	691.25	Joback Method
cpg	355.24	J/mol×K	728.82	Joback Method
cpg	364.95	J/mol×K	766.39	Joback Method
dvisc	0.0010425	Pa×s	338.76	Joback Method
dvisc	0.0007239	Pa×s	372.46	Joback Method
dvisc	0.0005341	Pa×s	406.16	Joback Method
dvisc	0.0004128	Pa×s	439.86	Joback Method
dvisc	0.0003310	Pa×s	473.56	Joback Method
dvisc	0.0002733	Pa×s	507.26	Joback Method
dvisc	0.0002311	Pa×s	540.96	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	385.20	K	0.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35587e+01
Coeff. B	-3.90043e+03
Coeff. C	-8.28420e+01
Temperature range (K), min.	376.75
Temperature range (K), max.	555.78

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1646533&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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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