Benzene, 1,4-dibromo-2-methyl-

Other names: 2,5-Dibromotoluene
Toluene, 2,5-dibromo-
Inchi: InChI=1S/C7H6Br2/c1-5-4-6(8)2-3-7(5)9/h2-4H,1H3
InchiKey: QKEZTJYRBHOKHH-UHFFFAOYSA-N
Formula: C7H6Br2
SMILES: Cc1cc(Br)ccc1Br
Mol. weight [g/mol]: 249.93
CAS: 615-59-8

Physical Properties

Property code	Value	Unit	Source
gf	129.85	kJ/mol	Joback Method
hf	78.44	kJ/mol	Joback Method
hfus	17.72	kJ/mol	Joback Method
hvap	47.65	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	3.520		Crippen Method
mcvol	120.730	ml/mol	McGowan Method
pc	4749.69	kPa	Joback Method
tb	509.20	K	NIST Webbook
tc	781.02	K	Joback Method
tf	278.77 ± 1.00	K	NIST Webbook
vc	0.444	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.12	J/mol×K	528.52	Joback Method
cpg	212.22	J/mol×K	570.60	Joback Method
cpg	220.62	J/mol×K	612.69	Joback Method
cpg	228.36	J/mol×K	654.77	Joback Method
cpg	235.51	J/mol×K	696.85	Joback Method
cpg	242.11	J/mol×K	738.94	Joback Method
cpg	248.21	J/mol×K	781.02	Joback Method

dvisc	0.0014758	Pa×s	339.71	Joback Method
dvisc	0.0010226	Pa×s	371.18	Joback Method
dvisc	0.0007504	Pa×s	402.65	Joback Method
dvisc	0.0005759	Pa×s	434.12	Joback Method
dvisc	0.0004581	Pa×s	465.58	Joback Method
dvisc	0.0003751	Pa×s	497.05	Joback Method
dvisc	0.0003145	Pa×s	528.52	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.70	K	4.70	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C615598&Units=SI
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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume