Benzene, 1,3-dibromo-5-methyl-

Other names:	1,3 Dibromo -5-methyl benzene
	3,5-Dibromotoluene
	Toluene, 3,5-dibromo-
Inchi:	InChI=1S/C7H6Br2/c1-5-2-6(8)4-7(9)3-5/h2-4H,1H3
InchiKey:	DPKKOVGCHDUSAI-UHFFFAOYSA-N
Formula:	C7H6Br2
SMILES:	Cc1cc(Br)cc(Br)c1
Mol. weight [g/mol]:	249.93
CAS:	1611-92-3

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	519.20	K	NIST Webbook
tc	781.02	K	Joback Method
tf	339.71	K	Joback Method
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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39603e+01
Coeff. B	-4.05185e+03
Coeff. C	-8.54740e+01
Temperature range (K), min.	381.82
Temperature range (K), max.	553.96

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=C1611923&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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