

Benzene, 1,2,4-tribromo-5-methyl-

Other names:	2,4,5-Tribromotoluene
Inchi:	InChI=1S/C7H5Br3/c1-4-2-6(9)7(10)3-5(4)8/h2-3H,1H3
InchiKey:	KZZJNNUPNNBCCH-UHFFFAOYSA-N
Formula:	C7H5Br3
SMILES:	Cc1cc(Br)c(Br)cc1Br
Mol. weight [g/mol]:	328.83
CAS:	3278-88-4

Physical Properties

Property code	Value	Unit	Source
gf	134.54	kJ/mol	Joback Method
hf	93.30	kJ/mol	Joback Method
hfus	22.62	kJ/mol	Joback Method
hvap	54.74	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	4.283		Crippen Method
mcvol	138.230	ml/mol	McGowan Method
pc	5123.98	kPa	Joback Method
tb	599.66	K	Joback Method
tc	868.00	K	Joback Method
tf	412.03	K	Joback Method
vc	0.505	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.22	J/molxK	599.66	Joback Method
cpg	235.92	J/molxK	644.38	Joback Method
cpg	242.99	J/molxK	689.11	Joback Method
cpg	249.48	J/molxK	733.83	Joback Method
cpg	255.47	J/molxK	778.55	Joback Method
cpg	261.03	J/molxK	823.28	Joback Method
cpg	266.22	J/molxK	868.00	Joback Method
dvisc	0.0010479	Paxs	412.03	Joback Method

dvisc	0.0007828	Paxs	443.30	Joback Method
dvisc	0.0006077	Paxs	474.57	Joback Method
dvisc	0.0004868	Paxs	505.84	Joback Method
dvisc	0.0004001	Paxs	537.12	Joback Method
dvisc	0.0003360	Paxs	568.39	Joback Method
dvisc	0.0002874	Paxs	599.66	Joback Method

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=C3278884&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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