

2,4-dibromotoluene

Inchi:	InChI=1S/C7H6Br2/c1-5-2-3-6(8)4-7(5)9/h2-4H,1H3
InchiKey:	GHWYNNFPUGEYEM-UHFFFAOYSA-N
Formula:	C7H6Br2
SMILES:	Cc1ccc(Br)cc1Br
Mol. weight [g/mol]:	249.93
CAS:	31543-75-6

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	528.52	K	Joback Method
tc	781.02	K	Joback Method
tf	263.45 ± 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/molxK	528.52	Joback Method
cpg	212.22	J/molxK	570.60	Joback Method
cpg	220.62	J/molxK	612.69	Joback Method
cpg	228.36	J/molxK	654.77	Joback Method
cpg	235.51	J/molxK	696.85	Joback Method
cpg	242.11	J/molxK	738.94	Joback Method
cpg	248.21	J/molxK	781.02	Joback Method
dvisc	0.0014758	Paxs	339.71	Joback Method
dvisc	0.0010226	Paxs	371.18	Joback Method

dvisc	0.0007504	Paxs	402.65	Joback Method
dvisc	0.0005759	Paxs	434.12	Joback Method
dvisc	0.0004581	Paxs	465.58	Joback Method
dvisc	0.0003751	Paxs	497.05	Joback Method
dvisc	0.0003145	Paxs	528.52	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31543756&Units=SI
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

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
mccvol:	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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