

2,3,5,6-Tetrabromo-p-xylene

Other names:	1,2,4,5-tetrabromodimethylbenzene 1,4-Bis(dibromomethyl)benzen Benzene, 1,2,4,5-tetrabromo-3,6-dimethyl- Tetrabromo-p-xylen Tetrabromo-p-xylene p-Tbx
Inchi:	InChI=1S/C8H6Br4/c1-3-5(9)7(11)4(2)8(12)6(3)10/h1-2H3
InchiKey:	RXKOKVQKECXOT-UHFFFAOYSA-N
Formula:	C8H6Br4
SMILES:	<chem>Cc1c(Br)c(Br)c(C)c(Br)c1Br</chem>
Mol. weight [g/mol]:	421.75
CAS:	23488-38-2

Physical Properties

Property code	Value	Unit	Source
chs	-3920.77	kJ/mol	NIST Webbook
gf	138.02	kJ/mol	Joback Method
hf	76.05	kJ/mol	Joback Method
hfus	29.71	kJ/mol	Joback Method
hvap	64.73	kJ/mol	Joback Method
log10ws	-7.07		Crippen Method
logp	5.353		Crippen Method
mcvol	169.820	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
tb	698.66	K	Joback Method
tc	973.89	K	Joback Method
tf	527.40	K	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	292.98	J/molxK	698.66	Joback Method
cpg	325.89	J/molxK	928.02	Joback Method
cpg	320.05	J/molxK	882.15	Joback Method
cpg	313.91	J/molxK	836.27	Joback Method
cpg	307.40	J/molxK	790.40	Joback Method
cpg	300.45	J/molxK	744.53	Joback Method
cpg	331.50	J/molxK	973.89	Joback Method
dvisc	0.0002157	Paxs	698.66	Joback Method
dvisc	0.0002469	Paxs	666.91	Joback Method
dvisc	0.0002864	Paxs	635.15	Joback Method
dvisc	0.0003374	Paxs	603.40	Joback Method
dvisc	0.0004049	Paxs	571.65	Joback Method
dvisc	0.0004963	Paxs	539.89	Joback Method
dvisc	0.0006242	Paxs	508.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23488382&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement of Vapor Pressures and Melting Properties of Five Polyaromatic Aromatic Flame Retardants:	https://www.doi.org/10.1021/acs.jced.7b01040 https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
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
mvol:	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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