2,3,5,6-TETRABROMO-P-XYLENE

Other names:	1,2,4,5-tetrabromodimethylbenzene
	1,4-Bis(dibrommethyl)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:	RXKOKVQKECXYOT-UHFFFAOYSA-N
Formula:	C8H6Br4
SMILES:	Cc1c(Br)c(Br)c(C)c(Br)c1Br
Mol. weight [g/mol]:	421.75

Physical Properties

Property code	Value	Unit	Source
af	0.4895		Cheméo Relay (1.0)
hf	121.43	kJ/mol	Cheméo Relay (1.0)
hfus	29.71	kJ/mol	Joback Method
hvap	73.07	kJ/mol	Cheméo Relay (1.0)
ie	8.42	eV	Cheméo Relay (1.0)
log10ws	-7.63		Cheméo Relay (1.0)
logp	5.353		Crippen Method
mcvol	169.820	ml/mol	McGowan Method
pc	4730.11	kPa	Joback Method
tb	615.93	K	Cheméo Relay (1.0)
tc	811.37	K	Cheméo Relay (1.0)
tf	527.40	K	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants
vc	0.570	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	292.98	J/mol×K	698.66	Joback Method
cpg	300.45	J/mol×K	744.53	Joback Method
cpg	307.40	J/mol×K	790.40	Joback Method
cpg	313.91	J/mol×K	836.27	Joback Method
cpg	320.05	J/mol×K	882.15	Joback Method
cpg	325.89	J/mol×K	928.02	Joback Method
cpg	331.50	J/mol×K	973.89	Joback Method
dvisc	0.0006242	Pa×s	508.14	Joback Method
dvisc	0.0004963	Pa×s	539.89	Joback Method
dvisc	0.0004049	Pa×s	571.65	Joback Method
dvisc	0.0003374	Pa×s	603.40	Joback Method
dvisc	0.0002864	Pa×s	635.15	Joback Method
dvisc	0.0002469	Pa×s	666.91	Joback Method
dvisc	0.0002157	Pa×s	698.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23488382&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants:	https://www.doi.org/10.1021/acs.jced.7b01040

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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