Benzene, pentabromomethyl-

Other names:	2,3,4,5,6-Pentabromotoluene
	FR-705
	Flammex 5BT
	Pentabromomethylbenzene
	Pentabromotoluene
	Toluene, 2,3,4,5,6-pentabromo-
Inchi:	InChI=1S/C7H3Br5/c1-2-3(8)5(10)7(12)6(11)4(2)9/h1H3
InchiKey:	OZHJEQVYCBTHJT-UHFFFAOYSA-N
Formula:	C7H3Br5
SMILES:	Cc1c(Br)c(Br)c(Br)c(Br)c1Br
Mol. weight [g/mol]:	486.62
CAS:	87-83-2

Physical Properties

Property code	Value	Unit	Source
gf	143.92	kJ/mol	Joback Method
hf	123.02	kJ/mol	Joback Method
hfus	32.41	kJ/mol	Joback Method
hvap	68.94	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	5.808		Crippen Method
mcvol	173.230	ml/mol	McGowan Method
pc	6018.58	kPa	Joback Method
tb	741.94	K	Joback Method
tc	1034.95	K	Joback Method
tf	559.00	K	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	266.69	J/mol×K	741.94	Joback Method
cpg	271.97	J/mol×K	790.77	Joback Method
cpg	276.92	J/mol×K	839.61	Joback Method
cpg	281.64	J/mol×K	888.44	Joback Method
cpg	286.23	J/mol×K	937.28	Joback Method
cpg	290.79	J/mol×K	986.11	Joback Method
cpg	295.41	J/mol×K	1034.95	Joback Method
dvisc	0.0005249	Pa×s	556.67	Joback Method
dvisc	0.0004276	Pa×s	587.55	Joback Method
dvisc	0.0003556	Pa×s	618.43	Joback Method
dvisc	0.0003009	Pa×s	649.31	Joback Method
dvisc	0.0002586	Pa×s	680.18	Joback Method
dvisc	0.0002251	Pa×s	711.06	Joback Method
dvisc	0.0001983	Pa×s	741.94	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87832&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants:	https://www.doi.org/10.1021/acs.jced.7b01040
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume