

pentabromoethylbenzene

Inchi:	InChI=1S/C8H5Br5/c1-2-3-4(9)6(11)8(13)7(12)5(3)10/h2H2,1H3
InchiKey:	FIAXCDIQXHJNIX-UHFFFAOYSA-N
Formula:	C8H5Br5
SMILES:	CCc1c(Br)c(Br)c(Br)c(Br)c1Br
Mol. weight [g/mol]:	500.65

Physical Properties

Property code	Value	Unit	Source
gf	152.34	kJ/mol	Joback Method
hf	102.38	kJ/mol	Joback Method
hfus	13.40	kJ/mol	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants
hvap	71.16	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	6.062		Crippen Method
mcvol	187.320	ml/mol	McGowan Method
pc	5213.15	kPa	Joback Method
tb	764.82	K	Joback Method
tc	1049.89	K	Joback Method
tf	408.90	K	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.82	J/molxK	907.35	Joback Method
cpg	320.94	J/molxK	812.33	Joback Method
cpg	314.47	J/molxK	764.82	Joback Method
cpg	338.43	J/molxK	954.86	Joback Method
cpg	343.96	J/molxK	1002.38	Joback Method

cpg	349.50	J/molxK	1049.89	Joback Method
cpg	327.02	J/molxK	859.84	Joback Method
dvisc	0.0003889	Paxs	600.75	Joback Method
dvisc	0.0003199	Paxs	633.57	Joback Method
dvisc	0.0002683	Paxs	666.38	Joback Method
dvisc	0.0002287	Paxs	699.19	Joback Method
dvisc	0.0001978	Paxs	732.01	Joback Method
dvisc	0.0004835	Paxs	567.94	Joback Method
dvisc	0.0001732	Paxs	764.82	Joback Method
psub	3.20e-04	kPa	367.30	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants
psub	2.10e-04	kPa	362.30	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants
psub	1.30e-04	kPa	357.40	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants
psub	8.30e-05	kPa	352.30	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants
psub	4.90e-05	kPa	347.40	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants
psub	3.20e-05	kPa	342.40	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants
psub	1.70e-05	kPa	337.50	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants

psub	1.04e-05	kPa	332.60	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants
psub	6.10e-06	kPa	327.60	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants
psub	3.70e-06	kPa	322.70	Measurement of Vapor Pressures and Melting Properties of Five Polybrominated Aromatic Flame Retardants

Sources

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
psub:	Sublimation pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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