

1,2,3,4,6,7,8-heptabromo-dibenzo-dioxin

Inchi:	InChI=1S/C12HBr7O2/c13-2-1-3-10(7(17)4(2)14)21-12-9(19)6(16)5(15)8(18)11(12)20-3/
InchiKey:	FPCROEVBHPWKPI-UHFFFAOYSA-N
Formula:	C12HBr7O2
SMILES:	BrC1cc2c(c(Br)c1Br)Oc1c(Br)c(Br)c(Br)c(Br)c1O2
Mol. weight [g/mol]:	736.46

Physical Properties

Property code	Value	Unit	Source
gf	196.87	kJ/mol	Joback Method
hf	98.43	kJ/mol	Joback Method
hfus	63.53	kJ/mol	Joback Method
hvap	106.93	kJ/mol	Joback Method
log10ws	-11.13		Crippen Method
logp	8.922		Crippen Method
mcvol	255.800	ml/mol	McGowan Method
pc	6503.64	kPa	Joback Method
rinpol	3924.00		NIST Webbook
rinpol	3924.00		NIST Webbook
tb	1096.30	K	Joback Method
tc	1414.46	K	Joback Method
tf	887.96	K	Joback Method
vc	0.933	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.44	J/molxK	1096.30	Joback Method
cpg	473.72	J/molxK	1149.33	Joback Method
cpg	485.57	J/molxK	1202.35	Joback Method
cpg	499.30	J/molxK	1255.38	Joback Method
cpg	515.21	J/molxK	1308.40	Joback Method
cpg	533.61	J/molxK	1361.43	Joback Method
cpg	554.79	J/molxK	1414.46	Joback Method
dvisc	0.0003189	Paxs	887.96	Joback Method

dvisc	0.0002807	Paxs	922.68	Joback Method
dvisc	0.0002494	Paxs	957.41	Joback Method
dvisc	0.0002234	Paxs	992.13	Joback Method
dvisc	0.0002016	Paxs	1026.85	Joback Method
dvisc	0.0001831	Paxs	1061.58	Joback Method
dvisc	0.0001674	Paxs	1096.30	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172304&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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