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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0002807	Pa×s	922.68	Joback Method
dvisc	0.0002494	Pa×s	957.41	Joback Method
dvisc	0.0002234	Pa×s	992.13	Joback Method
dvisc	0.0002016	Pa×s	1026.85	Joback Method
dvisc	0.0001831	Pa×s	1061.58	Joback Method
dvisc	0.0001674	Pa×s	1096.30	Joback Method

Sources

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
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
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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