

1,2,6,9-tetrabromo-dibenzo-dioxin

Inchi:	InChI=1S/C12H4Br4O2/c13-5-3-4-8-12(9(5)16)18-11-7(15)2-1-6(14)10(11)17-8/h1-4H
InchiKey:	AXQIJJXLM DHTLJ-UHFFFAOYSA-N
Formula:	C12H4Br4O2
SMILES:	BrC1ccc2c(c1Br)Oc1c(Br)ccc(Br)c1O2
Mol. weight [g/mol]:	499.77

Physical Properties

Property code	Value	Unit	Source
gf	182.80	kJ/mol	Joback Method
hf	53.85	kJ/mol	Joback Method
hfus	48.85	kJ/mol	Joback Method
hvap	85.64	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.635		Crippen Method
mvol	203.300	ml/mol	McGowan Method
pc	5087.49	kPa	Joback Method
rinpol	2826.00		NIST Webbook
rinpol	2826.00		NIST Webbook
tb	882.88	K	Joback Method
tc	1180.48	K	Joback Method
tf	671.00	K	Joback Method
vc	0.748	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.07	J/molxK	882.88	Joback Method
cpg	419.55	J/molxK	932.48	Joback Method
cpg	427.01	J/molxK	982.08	Joback Method
cpg	434.69	J/molxK	1031.68	Joback Method
cpg	442.80	J/molxK	1081.28	Joback Method
cpg	451.58	J/molxK	1130.88	Joback Method
cpg	461.26	J/molxK	1180.48	Joback Method
dvisc	0.0008138	Paxs	671.00	Joback Method

dvisc	0.0006851	Paxs	706.31	Joback Method
dvisc	0.0005863	Paxs	741.63	Joback Method
dvisc	0.0005088	Paxs	776.94	Joback Method
dvisc	0.0004471	Paxs	812.25	Joback Method
dvisc	0.0003971	Paxs	847.57	Joback Method
dvisc	0.0003561	Paxs	882.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172384&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mccvol:	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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