1,3-dibromo-dibenzo-dioxin

Inchi: InChI=1S/C12H6Br2O2/c13-7-5-8(14)12-11(6-7)15-9-3-1-2-4-10(9)16-12/h1-6H
InchiKey: CEMPIZJFPAOXRG-UHFFFAOYSA-N
Formula: C12H6Br2O2
SMILES: Brc1cc(Br)c2c(c1)Oc1ccccc1O2
Mol. weight [g/mol]: 341.98

Physical Properties

Property code	Value	Unit	Source
gf	173.42	kJ/mol	Joback Method
hf	24.13	kJ/mol	Joback Method
hfus	39.05	kJ/mol	Joback Method
hvap	71.45	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	5.110		Crippen Method
mcvol	168.300	ml/mol	McGowan Method
pc	4385.77	kPa	Joback Method
rinpol	2112.00		NIST Webbook
rinpol	2112.00		NIST Webbook
tb	740.60	K	Joback Method
tc	1020.08	K	Joback Method
tf	526.36	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.39	J/mol×K	740.60	Joback Method
cpg	381.75	J/mol×K	787.18	Joback Method
cpg	390.37	J/mol×K	833.76	Joback Method
cpg	398.41	J/mol×K	880.34	Joback Method
cpg	406.06	J/mol×K	926.92	Joback Method
cpg	413.49	J/mol×K	973.50	Joback Method
cpg	420.88	J/mol×K	1020.08	Joback Method
dvisc	0.0013795	Pa×s	526.36	Joback Method

dvisc	0.0011043	Pa×s	562.07	Joback Method
dvisc	0.0009077	Pa×s	597.77	Joback Method
dvisc	0.0007629	Pa×s	633.48	Joback Method
dvisc	0.0006531	Pa×s	669.19	Joback Method
dvisc	0.0005680	Pa×s	704.89	Joback Method
dvisc	0.0005007	Pa×s	740.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172522&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