2-bromo-dibenzo-dioxin

Inchi: InChI=1S/C12H7BrO2/c13-8-5-6-11-12(7-8)15-10-4-2-1-3-9(10)14-11/h1-7H
InchiKey: GSUCEGNAROQSGU-UHFFFAOYSA-N
Formula: C12H7BrO2
SMILES: Brc1ccc2c(c1)Oc1ccccc1O2
Mol. weight [g/mol]: 263.09

Physical Properties

Property code	Value	Unit	Source
gf	168.73	kJ/mol	Joback Method
hf	9.27	kJ/mol	Joback Method
hfus	34.16	kJ/mol	Joback Method
hvap	64.35	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	4.347		Crippen Method
mcvol	150.800	ml/mol	McGowan Method
pc	4088.15	kPa	Joback Method
rinpol	1880.00		NIST Webbook
tb	669.46	K	Joback Method
tc	937.67	K	Joback Method
tf	454.04	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.20	J/mol×K	669.46	Joback Method
cpg	393.98	J/mol×K	892.97	Joback Method
cpg	386.03	J/mol×K	848.27	Joback Method
cpg	377.53	J/mol×K	803.57	Joback Method
cpg	368.32	J/mol×K	758.86	Joback Method
cpg	358.26	J/mol×K	714.16	Joback Method
cpg	401.52	J/mol×K	937.67	Joback Method
dvisc	0.0005411	Pa×s	669.46	Joback Method
dvisc	0.0006201	Pa×s	633.56	Joback Method

dvisc	0.0007224	Pa×s	597.65	Joback Method
dvisc	0.0008582	Pa×s	561.75	Joback Method
dvisc	0.0010437	Pa×s	525.85	Joback Method
dvisc	0.0013063	Pa×s	489.94	Joback Method
dvisc	0.0016940	Pa×s	454.04	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R172859&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