Benzofuranone, 2(3h)-, 3-(2,3-dibromopropyl)-3-phenyl

Other names: Benzofuranone, 2(3h)-,3-(2',3'-dibromoproypyl)-3-phenyl-,
Inchi: InChI=1S/C17H14Br2O2/c18-11-13(19)10-17(12-6-2-1-3-7-12)14-8-4-5-9-15(14)21-16(1
InchiKey: FKSMJSVUWKOPCJ-UHFFFAOYSA-N
Formula: C17H14Br2O2
SMILES: O=C1Oc2ccccc2C1(CC(Br)CBr)c1ccccc1
Mol. weight [g/mol]: 410.10
CAS: 93319-87-0

Physical Properties

Property code	Value	Unit	Source
gf	180.20	kJ/mol	Joback Method
hf	-66.90	kJ/mol	Joback Method
hfus	33.85	kJ/mol	Joback Method
hvap	78.65	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.440		Crippen Method
mcvol	234.450	ml/mol	McGowan Method
pc	2902.98	kPa	Joback Method
tb	880.33	K	Joback Method
tc	1161.46	K	Joback Method
tf	587.94	K	Joback Method
vc	0.873	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	638.43	J/mol×K	880.33	Joback Method
cpg	654.85	J/mol×K	927.18	Joback Method
cpg	671.36	J/mol×K	974.04	Joback Method
cpg	688.32	J/mol×K	1020.89	Joback Method
cpg	706.06	J/mol×K	1067.75	Joback Method
cpg	724.94	J/mol×K	1114.60	Joback Method
cpg	745.29	J/mol×K	1161.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C93319870&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume