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

Inchi: InChI=1S/C17H15BrO2/c18-12-6-11-17(13-7-2-1-3-8-13)14-9-4-5-10-15(14)20-16(17)19/

InchiKey: GUZOMDMCWOJYEU-UHFFFAOYSA-N

Formula: C17H15BrO2

SMILES: O=C1Oc2ccccc2C1(CCCBr)c1ccccc1

Mol. weight [g/mol]: 331.20

CAS: 93323-03-6

Physical Properties

Property code	Value	Unit	Source
gf	168.32	kJ/mol	Joback Method
hf	-87.95	kJ/mol	Joback Method
hfus	32.09	kJ/mol	Joback Method
hvap	72.60	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.067		Crippen Method
mcvol	216.950	ml/mol	McGowan Method
pc	2676.31	kPa	Joback Method
tb	814.61	K	Joback Method
tc	1082.40	K	Joback Method
tf	543.14	K	Joback Method
vc	0.817	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.81	J/mol×K	814.61	Joback Method
cpg	620.34	J/mol×K	859.24	Joback Method
cpg	636.46	J/mol×K	903.87	Joback Method
cpg	652.44	J/mol×K	948.51	Joback Method
cpg	668.56	J/mol×K	993.14	Joback Method
cpg	685.12	J/mol×K	1037.77	Joback Method
cpg	702.38	J/mol×K	1082.40	Joback Method

Sources

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=C93323036&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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