Furan-2(3h)-one, 5-(bromomethyl)-4,5-dihydro-3-(o-hydroxyphenyl)-3

Inchi: InChI=1S/C17H15BrO3/c18-11-13-10-17(16(20)21-13,12-6-2-1-3-7-12)14-8-4-5-9-15(14)

InchiKey: RBRMYLBOSHCYII-UHFFFAOYSA-N

Formula: C17H15BrO3

SMILES: O=C1OC(CBr)CC1(c1ccccc1)c1ccccc1O

Mol. weight [g/mol]: 347.20

CAS: 94574-85-3

Physical Properties

Property code	Value	Unit	Source
gf	-8.58	kJ/mol	Joback Method
hf	-286.45	kJ/mol	Joback Method
hfus	35.13	kJ/mol	Joback Method
hvap	84.99	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.389		Crippen Method
mcvol	222.820	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
tb	894.12	K	Joback Method
tc	1181.48	K	Joback Method
tf	631.06	K	Joback Method
vc	0.765	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.98	J/mol×K	894.12	Joback Method
cpg	684.27	J/mol×K	942.01	Joback Method
cpg	702.78	J/mol×K	989.91	Joback Method
cpg	721.92	J/mol×K	1037.80	Joback Method
cpg	742.06	J/mol×K	1085.69	Joback Method
cpg	763.61	J/mol×K	1133.58	Joback Method
cpg	786.96	J/mol×K	1181.48	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=C94574853&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