Benzofuranone, 2(3h)-, 3-(beta-benzyloxyethyl)-3-phenyl-

Inchi: InChI=1S/C23H20O3/c24-22-23(19-11-5-2-6-12-19,20-13-7-8-14-21(20)26-22)15-16-25-
InchiKey: HKFUMYMRIDLVFH-UHFFFAOYSA-N
Formula: C23H20O3
SMILES: O=C1Oc2ccccc2C1(CCOCc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 344.40
CAS: 95435-96-4

Physical Properties

Property code	Value	Unit	Source
gf	211.93	kJ/mol	Joback Method
hf	-133.81	kJ/mol	Joback Method
hfus	37.57	kJ/mol	Joback Method
hvap	84.21	kJ/mol	Joback Method
log10ws	-5.49		Crippen Method
logp	4.499		Crippen Method
mcvol	266.100	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
tb	934.83	K	Joback Method
tc	1200.14	K	Joback Method
tf	599.61	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.22	J/mol×K	934.83	Joback Method
cpg	862.50	J/mol×K	979.05	Joback Method
cpg	881.51	J/mol×K	1023.27	Joback Method
cpg	900.55	J/mol×K	1067.48	Joback Method
cpg	919.87	J/mol×K	1111.70	Joback Method
cpg	939.77	J/mol×K	1155.92	Joback Method
cpg	960.52	J/mol×K	1200.14	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=C95435964&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

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