4-(2-phenylethoxy)-«gamma»-valerolactone

Inchi: InChI=1S/C13H16O3/c1-10-12(9-13(14)16-10)15-8-7-11-5-3-2-4-6-11/h2-6,10,12H,7-9H2
InchiKey: OHNBWRNLOPMBAN-UHFFFAOYSA-N
Formula: C13H16O3
SMILES: CC1OC(=O)CC1OCCc1ccccc1
Mol. weight [g/mol]: 220.26

Physical Properties

Property code	Value	Unit	Source
gf	-113.88	kJ/mol	Joback Method
hf	-436.90	kJ/mol	Joback Method
hfus	27.15	kJ/mol	Joback Method
hvap	57.92	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.950		Crippen Method
mcvol	172.720	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
ripol	2667.00		NIST Webbook
ripol	2667.00		NIST Webbook
tb	651.32	K	Joback Method
tc	886.07	K	Joback Method
tf	386.37	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.99	J/mol×K	651.32	Joback Method
cpg	495.59	J/mol×K	690.44	Joback Method
cpg	512.93	J/mol×K	729.57	Joback Method
cpg	529.01	J/mol×K	768.69	Joback Method
cpg	543.85	J/mol×K	807.82	Joback Method
cpg	557.44	J/mol×K	846.94	Joback Method
cpg	569.77	J/mol×K	886.07	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=R321407&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume