4-(phenylmethoxy)-«gamma»-valerolactone

Inchi: InChI=1S/C12H14O3/c1-9-11(7-12(13)15-9)14-8-10-5-3-2-4-6-10/h2-6,9,11H,7-8H2,1H3
InchiKey: AKWGWVSTXAZVAU-UHFFFAOYSA-N
Formula: C12H14O3
SMILES: CC1OC(=O)CC1OCc1ccccc1
Mol. weight [g/mol]: 206.24

Physical Properties

Property code	Value	Unit	Source
gf	-122.30	kJ/mol	Joback Method
hf	-416.26	kJ/mol	Joback Method
hfus	24.56	kJ/mol	Joback Method
hvap	55.70	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	1.907		Crippen Method
mcvol	158.630	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
ripol	2616.00		NIST Webbook
tb	628.44	K	Joback Method
tc	868.13	K	Joback Method
tf	375.10	K	Joback Method
vc	0.586	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.27	J/mol×K	628.44	Joback Method
cpg	443.42	J/mol×K	668.39	Joback Method
cpg	460.35	J/mol×K	708.34	Joback Method
cpg	476.07	J/mol×K	748.28	Joback Method
cpg	490.58	J/mol×K	788.23	Joback Method
cpg	503.86	J/mol×K	828.18	Joback Method
cpg	515.92	J/mol×K	868.13	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=R321447&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