3-Pentyl-4,5-dihydroisobenzofuran-1(3H)-one

Inchi: InChI=1S/C13H18O2/c1-2-3-4-9-12-10-7-5-6-8-11(10)13(14)15-12/h6,8,12H,2-5,7,9H2,1
InchiKey: LSRBNNXNGNVZQN-UHFFFAOYSA-N
Formula: C13H18O2
SMILES: CCCCCC1OC(=O)C2=C1CCC=C2
Mol. weight [g/mol]: 206.28
CAS: 128575-99-5

Physical Properties

Property code	Value	Unit	Source
gf	-16.56	kJ/mol	Joback Method
hf	-341.27	kJ/mol	Joback Method
hfus	27.48	kJ/mol	Joback Method
hvap	55.85	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.139		Crippen Method
mcvol	171.150	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	1792.50		NIST Webbook
rinpol	1792.50		NIST Webbook
tb	630.85	K	Joback Method
tc	852.67	K	Joback Method
tf	387.18	K	Joback Method
vc	0.654	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	465.58	J/mol×K	630.85	Joback Method
cpg	483.19	J/mol×K	667.82	Joback Method
cpg	499.73	J/mol×K	704.79	Joback Method
cpg	515.25	J/mol×K	741.76	Joback Method
cpg	529.79	J/mol×K	778.73	Joback Method
cpg	543.37	J/mol×K	815.70	Joback Method
cpg	556.04	J/mol×K	852.67	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=C128575995&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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