(S)-4-Methoxy-6-phenethyl-5,6-dihydro-2H-pyran-2

Inchi: InChI=1S/C14H16O3/c1-16-13-9-12(17-14(15)10-13)8-7-11-5-3-2-4-6-11/h2-6,10,12H,7-

InchiKey: VOOYTQRREPYRIW-GFCCVEGCSA-N

Formula: C14H16O3

SMILES: COC1=CC(=O)OC(CCc2ccccc2)C1

Mol. weight [g/mol]: 232.28

CAS: 587-63-3

Physical Properties

Property code	Value	Unit	Source
gf	-89.52	kJ/mol	Joback Method
hf	-397.05	kJ/mol	Joback Method
hfus	27.40	kJ/mol	Joback Method
hvap	61.58	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.465		Crippen Method
mcvol	182.510	ml/mol	McGowan Method
pc	2510.03	kPa	Joback Method
rinpol	2168.10		NIST Webbook
rinpol	2168.10		NIST Webbook
tb	687.28	K	Joback Method
tc	927.69	K	Joback Method
tf	411.64	K	Joback Method
vc	0.676	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.08	J/mol×K	687.28	Joback Method
cpg	524.08	J/mol×K	727.35	Joback Method
cpg	540.75	J/mol×K	767.42	Joback Method
cpg	556.07	J/mol×K	807.49	Joback Method
cpg	570.06	J/mol×K	847.55	Joback Method
cpg	582.70	J/mol×K	887.62	Joback Method
cpg	593.99	J/mol×K	927.69	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=C587633&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume