Thiopyran-3-carboxylic acid, 5-benzamido-4-oxo-, ethyl ester

Inchi: InChI=1S/C15H17NO4S/c1-2-20-15(19)11-8-21-9-12(13(11)17)16-14(18)10-6-4-3-5-7-10

InchiKey: CDIUBHOIPBTGSZ-UHFFFAOYSA-N

Formula: C15H17NO4S

SMILES: CCOC(=O)C1CSCC(N=C(O)c2ccccc2)C1=O

Mol. weight [g/mol]: 307.37

CAS: 116277-58-8

Physical Properties

Property code	Value	Unit	Source
hf	-499.46	kJ/mol	Joback Method
hvap	90.67	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.855		Crippen Method
mcvol	224.500	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
tb	944.84	K	Joback Method
tc	1191.06	K	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=C116277588&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf: Enthalpy of formation 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