

Butric acid, 2-benzamido-4[(carboxymethyl)thio]-, dimethyl ester

InChI: InChI=1S/C15H19NO5S/c1-20-13(17)10-22-9-8-12(15(19)21-2)16-14(18)11-6-4-3-5-7-11
InChIKey: BDJZYNKTSKRFLS-UHFFFAOYSA-N

Formula: C15H19NO5S
SMILES: COC(=O)CSCCC(N=C(O)c1ccccc1)C(=O)OC
Mol. weight [g/mol]: 325.38

Physical Properties

Property code	Value	Unit	Source
hf	-649.21	kJ/mol	Joback Method
hvap	96.07	kJ/mol	Joback Method
log10ws	-2.01		Crippen Method
logp	1.829		Crippen Method
mcvol	241.230	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
tb	958.94	K	Joback Method
tc	1186.60	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=B6008689&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

Latest version available from:

<https://www.cheméo.com/cid/85-091-7/Butric-acid-2-benzamido-4-carboxymethyl-thio-dimethyl-ester.pdf>

Generated by Cheméo on 2025-12-06 00:50:01.848653532 +0000 UTC m=+4730399.378694196.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.