L (-)-2-benzoylamino-1,4-butanediol dibenzoate

Inchi: InChI=1S/C25H23NO5/c27-23(19-10-4-1-5-11-19)26-22(18-31-25(29)21-14-8-3-9-15-21)
InchiKey: AAAWGJKZEIQYJT-UHFFFAOYSA-N
Formula: C25H23NO5
SMILES: O=C(OCCC(COC(=O)c1ccccc1)N=C(O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 417.45
CAS: 10405-09-1

Physical Properties

Property code	Value	Unit	Source
hf	-424.42	kJ/mol	Joback Method
hvap	116.07	kJ/mol	Joback Method
log10ws	-5.67		Crippen Method
logp	4.464		Crippen Method
mcvol	318.260	ml/mol	McGowan Method
pc	1558.58	kPa	Joback Method
tb	1172.32	K	Joback Method
tc	1436.15	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=C10405091&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