4,4'-Dithiobis(3-benzoylamino-1-butanol benzoate)

Inchi: InChI=1S/C36H36N2O6S2/c39-33(27-13-5-1-6-14-27)37-31(21-23-43-35(41)29-17-9-3-1
InchiKey: KWXMVCPLUPAUTP-UHFFFAOYSA-N
Formula: C36H36N2O6S2
SMILES: O=C(OCCC(CSSCC(CCOC(=O)c1ccccc1)N=C(O)c1ccccc1)N=C(O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 656.81
CAS: 96772-45-1

Physical Properties

Property code	Value	Unit	Source
hf	-416.27	kJ/mol	Joback Method
hvap	176.15	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	7.609		Crippen Method
mcvol	493.740	ml/mol	McGowan Method
pc	962.08	kPa	Joback Method
tb	1756.54	K	Joback Method
tc	2314.97	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C96772451&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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