L(-)-3-benzoylamino-4-benzoylmercapto-1-butano benzoate

Inchi: InChI=1S/C25H23NO4S/c27-23(19-10-4-1-5-11-19)26-22(18-31-25(29)21-14-8-3-9-15-2
InchiKey: TYKGHWYHOPGIRA-UHFFFAOYSA-N
Formula: C25H23NO4S
SMILES: O=C(NC(CCOC(=O)c1ccccc1)CSC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 433.52
CAS: 10357-55-8

Physical Properties

Property code	Value	Unit	Source
gf	125.16	kJ/mol	Joback Method
hf	-229.64	kJ/mol	Joback Method
hfus	54.32	kJ/mol	Joback Method
hvap	113.58	kJ/mol	Joback Method
log10ws	-6.93		Crippen Method
logp	4.606		Crippen Method
mcvol	328.740	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
tb	1153.98	K	Joback Method
tc	1421.64	K	Joback Method
tf	694.85	K	Joback Method
vc	1.230	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1040.72	J/mol×K	1153.98	Joback Method
cpg	1048.14	J/mol×K	1198.59	Joback Method
cpg	1054.27	J/mol×K	1243.20	Joback Method
cpg	1059.23	J/mol×K	1287.81	Joback Method
cpg	1063.16	J/mol×K	1332.42	Joback Method
cpg	1066.22	J/mol×K	1377.03	Joback Method
cpg	1068.53	J/mol×K	1421.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10357558&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume