Alpha,alpha'-diacetyl-3,3'-bis(trifluoromethyl) glutaranilide

Inchi: InChI=1S/C23H20F6N2O4/c1-12(32)18(20(34)30-16-7-3-5-14(9-16)22(24,25)26)11-19(1

InchiKey: HSTHVXVQGIFWNK-UHFFFAOYSA-N

Formula: C23H20F6N2O4

SMILES: CC(=O)C(CC(C(C)=O)C(O)=Nc1cccc(C(F)(F)F)c1)C(O)=Nc1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 502.41

CAS: 3870-70-0

Physical Properties

Property code	Value	Unit	Source
hf	-1657.41	kJ/mol	Joback Method
hvap	118.04	kJ/mol	Joback Method
log10ws	-6.27		Crippen Method
logp	6.401		Crippen Method
mcvol	324.270	ml/mol	McGowan Method
pc	1189.06	kPa	Joback Method
tb	1222.46	K	Joback Method
tc	1514.74	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3870700&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