Thio-o,o'-benzoic acid, diphenacyl ester

Inchi: InChI=1S/C30H22O6S/c31-25(21-11-3-1-4-12-21)19-35-29(33)23-15-7-9-17-27(23)37-28
InchiKey: YAOINMIXANHPKJ-UHFFFAOYSA-N
Formula: C30H22O6S
SMILES: O=C(COC(=O)c1ccccc1Sc1ccccc1C(=O)OCC(=O)c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 510.56
CAS: 116435-10-0

Physical Properties

Property code	Value	Unit	Source
gf	-60.46	kJ/mol	Joback Method
hf	-412.24	kJ/mol	Joback Method
hfus	61.74	kJ/mol	Joback Method
hvap	131.42	kJ/mol	Joback Method
log10ws	-8.15		Crippen Method
logp	5.917		Crippen Method
mcvol	372.890	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
tb	1331.58	K	Joback Method
tc	1630.61	K	Joback Method
tf	837.16	K	Joback Method
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1157.94	J/mol×K	1331.58	Joback Method
cpg	1157.53	J/mol×K	1381.42	Joback Method
cpg	1155.48	J/mol×K	1431.26	Joback Method
cpg	1151.95	J/mol×K	1481.09	Joback Method
cpg	1147.11	J/mol×K	1530.93	Joback Method
cpg	1141.13	J/mol×K	1580.77	Joback Method
cpg	1134.17	J/mol×K	1630.61	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=C116435100&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

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