Di-acetodiphenylmonosulfide

Inchi: InChI=1S/C16H14O2S/c1-11(17)13-3-7-15(8-4-13)19-16-9-5-14(6-10-16)12(2)18/h3-10H
InchiKey: JBDYORUCEWAWQR-UHFFFAOYSA-N
Formula: C16H14O2S
SMILES: CC(=O)c1ccc(Sc2ccc(C(C)=O)cc2)cc1
Mol. weight [g/mol]: 270.35
CAS: 2615-09-0

Physical Properties

Property code	Value	Unit	Source
gf	64.68	kJ/mol	Joback Method
hf	-106.74	kJ/mol	Joback Method
hfus	31.83	kJ/mol	Joback Method
hvap	77.39	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.243		Crippen Method
mcvol	208.270	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
tb	805.32	K	Joback Method
tc	1063.18	K	Joback Method
tf	482.22	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.22	J/mol×K	805.32	Joback Method
cpg	569.49	J/mol×K	848.30	Joback Method
cpg	581.44	J/mol×K	891.27	Joback Method
cpg	592.16	J/mol×K	934.25	Joback Method
cpg	601.69	J/mol×K	977.22	Joback Method
cpg	610.10	J/mol×K	1020.20	Joback Method
cpg	617.46	J/mol×K	1063.18	Joback Method

Sources

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=C2615090&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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