Acetic 3-(acetylsulfanyl)benzoic anhydride

Inchi: InChI=1S/C11H10O4S/c1-7(12)15-11(14)9-4-3-5-10(6-9)16-8(2)13/h3-6H,1-2H3
InchiKey: MHOVADNDAZLWCF-UHFFFAOYSA-N
Formula: C11H10O4S
SMILES: CC(=O)OC(=O)c1cccc(SC(C)=O)c1
Mol. weight [g/mol]: 238.26

Physical Properties

Property code	Value	Unit	Source
gf	-314.12	kJ/mol	Joback Method
hf	-473.40	kJ/mol	Joback Method
hfus	28.01	kJ/mol	Joback Method
hvap	72.48	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.029		Crippen Method
mcvol	169.020	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	1856.30		NIST Webbook
rinpol	1856.30		NIST Webbook
tb	735.55	K	Joback Method
tc	975.26	K	Joback Method
tf	459.09	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.69	J/mol×K	735.55	Joback Method
cpg	433.69	J/mol×K	775.50	Joback Method
cpg	443.71	J/mol×K	815.45	Joback Method
cpg	452.75	J/mol×K	855.41	Joback Method
cpg	460.83	J/mol×K	895.36	Joback Method
cpg	467.94	J/mol×K	935.31	Joback Method
cpg	474.08	J/mol×K	975.26	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=U352984&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume