4-(4-Acetoxy-5-tert-butyl-2-methylphenyl)sulfanyl-
acetate

Inchi: InChI=1S/C26H34O4S/c1-15-11-21(29-17(3)27)19(25(5,6)7)13-23(15)31-24-14-20(26(8,
InchiKey: HJVRTJOXJRZISJ-UHFFFAOYSA-N
Formula: C26H34O4S
SMILES: CC(=O)Oc1cc(C)c(Sc2cc(C(C)(C)C)c(OC(C)=O)cc2C)cc1C(C)(C)C
Mol. weight [g/mol]: 442.61
CAS: 32604-54-9

Physical Properties

Property code	Value	Unit	Source
gf	-93.96	kJ/mol	Joback Method
hf	-640.96	kJ/mol	Joback Method
hfus	43.72	kJ/mol	Joback Method
hvap	104.53	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	6.900		Crippen Method
mcvol	360.910	ml/mol	McGowan Method
pc	1114.82	kPa	Joback Method
rinpol	2870.00		NIST Webbook
tb	1092.42	K	Joback Method
tc	1343.23	K	Joback Method
tf	694.30	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1182.39	J/mol×K	1092.42	Joback Method
cpg	1194.32	J/mol×K	1134.22	Joback Method
cpg	1204.67	J/mol×K	1176.02	Joback Method
cpg	1213.51	J/mol×K	1217.83	Joback Method
cpg	1220.94	J/mol×K	1259.63	Joback Method
cpg	1227.02	J/mol×K	1301.43	Joback Method
cpg	1231.85	J/mol×K	1343.23	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=C32604549&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