3,7-Dimethyl-1-thiaindene sulfone

Inchi: InChI=1S/C10H10O2S/c1-7-4-3-5-9-8(2)6-13(11,12)10(7)9/h3-6H,1-2H3
InchiKey: OITNEHOYSPWFRO-UHFFFAOYSA-N
Formula: C10H10O2S
SMILES: CC1=CS(=O)(=O)c2c(C)cccc21
Mol. weight [g/mol]: 194.25
CAS: 42346-86-1

Physical Properties

Property code	Value	Unit	Source
chl	-5724.00 ± 92.00	kJ/mol	NIST Webbook
gf	-246.54	kJ/mol	Joback Method
hf	-346.65	kJ/mol	Joback Method
hfl	63.01	kJ/mol	NIST Webbook
hfus	23.72	kJ/mol	Joback Method
hvap	60.26	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.143		Crippen Method
mcvol	140.930	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
tb	507.22	K	Joback Method
tc	719.07	K	Joback Method
tf	376.99	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.18	J/mol×K	507.22	Joback Method
cpg	310.24	J/mol×K	542.53	Joback Method
cpg	322.46	J/mol×K	577.84	Joback Method
cpg	333.87	J/mol×K	613.14	Joback Method
cpg	344.51	J/mol×K	648.45	Joback Method
cpg	354.44	J/mol×K	683.76	Joback Method
cpg	363.70	J/mol×K	719.07	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=C42346861&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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