4-tert-Butyl-1(1-thioxo-2,2-dimethyl-propyl)-benze

Other names: 1-Propanethione, 1-[4-(1,1-dimethylethyl)phenyl]-2,2-dimethyl-
Inchi: InChI=1S/C15H22S/c1-14(2,3)12-9-7-11(8-10-12)13(16)15(4,5)6/h7-10H,1-6H3
InchiKey: ZPRFQKNKKXHCDW-UHFFFAOYSA-N
Formula: C15H22S
SMILES: CC(C)(C)C(=S)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]: 234.40
CAS: 72194-24-2

Physical Properties

Property code	Value	Unit	Source
gf	300.94	kJ/mol	Joback Method
hf	1.13	kJ/mol	Joback Method
hfus	18.03	kJ/mol	Joback Method
hvap	56.06	kJ/mol	Joback Method
ie	7.85	eV	NIST Webbook
ie	8.96	eV	NIST Webbook
log10ws	-5.06		Crippen Method
logp	4.748		Crippen Method
mcvol	210.500	ml/mol	McGowan Method
pc	2043.76	kPa	Joback Method
tb	637.84	K	Joback Method
tc	877.23	K	Joback Method
tf	336.86	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.24	J/mol×K	637.84	Joback Method
cpg	558.89	J/mol×K	677.74	Joback Method
cpg	576.07	J/mol×K	717.64	Joback Method
cpg	591.93	J/mol×K	757.54	Joback Method
cpg	606.65	J/mol×K	797.43	Joback Method
cpg	620.39	J/mol×K	837.33	Joback Method

cpg	633.28	J/mol×K	877.23	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=C72194242&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
ie:	Ionization energy
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