2,4-Di-tert-butylthiophenol

Inchi: InChI=1S/C14H22S/c1-13(2,3)10-7-8-12(15)11(9-10)14(4,5)6/h7-9,15H,1-6H3
InchiKey: ACJAQOIIEMFTGS-UHFFFAOYSA-N
Formula: C14H22S
SMILES: CC(C)(C)c1ccc(S)c(C(C)(C)C)c1
Mol. weight [g/mol]: 222.39
CAS: 19728-43-9

Physical Properties

Property code	Value	Unit	Source
gf	195.22	kJ/mol	Joback Method
hf	-97.72	kJ/mol	Joback Method
hfus	14.49	kJ/mol	Joback Method
hvap	54.50	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	4.570		Crippen Method
mcvol	200.710	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
tb	612.76	K	Joback Method
tc	853.10	K	Joback Method
tf	340.30	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	506.52	J/mol×K	612.76	Joback Method
cpg	525.96	J/mol×K	652.82	Joback Method
cpg	543.95	J/mol×K	692.87	Joback Method
cpg	560.60	J/mol×K	732.93	Joback Method
cpg	576.01	J/mol×K	772.99	Joback Method
cpg	590.30	J/mol×K	813.04	Joback Method
cpg	603.57	J/mol×K	853.10	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=C19728439&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