Methyl 4-tert-butyl-dithiabenzoate

Other names:	Methyl 4-tert-butylbenzenecarbodithioate
	Benzenecarbodithioic acid, 4-(1,1-dimethylethyl)-, methyl ester
Inchi:	InChI=1S/C12H16S2/c1-12(2,3)10-7-5-9(6-8-10)11(13)14-4/h5-8H,1-4H3
InchiKey:	XGVNDLXEGXTPBM-UHFFFAOYSA-N
Formula:	C12H16S2
SMILES:	CSC(=S)c1ccc(C(C)(C)C)cc1
Mol. weight [g/mol]:	224.38
CAS:	58863-42-6

Physical Properties

Property code	Value	Unit	Source
gf	305.96	kJ/mol	Joback Method
hf	113.67	kJ/mol	Joback Method
hfus	21.81	kJ/mol	Joback Method
hvap	57.49	kJ/mol	Joback Method
ie	8.03	eV	NIST Webbook
log10ws	-4.42		Crippen Method
logp	4.023		Crippen Method
mcvol	184.580	ml/mol	McGowan Method
pc	2695.80	kPa	Joback Method
tb	641.21	K	Joback Method
tc	899.57	K	Joback Method
tf	335.03	K	Joback Method
vc	0.678	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.27	J/mol×K	641.21	Joback Method
cpg	455.99	J/mol×K	684.27	Joback Method
cpg	470.40	J/mol×K	727.33	Joback Method
cpg	483.63	J/mol×K	770.39	Joback Method
cpg	495.81	J/mol×K	813.45	Joback Method
cpg	507.08	J/mol×K	856.51	Joback Method

cpg	517.58	J/mol×K	899.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C58863426&Units=SI
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

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