4-Tolyl chlorothionoformate

Other names:	O-p-Tolyl chlorothioformate
	p-Tolyl chlorothionoformate
	O-4-Methylphenyl chlorothioformate
	Carbonochloridothioic acid, O-(4-methylphenyl) ester
Inchi:	InChI=1S/C8H7ClOS/c1-6-2-4-7(5-3-6)10-8(9)11/h2-5H,1H3
InchiKey:	UNCAXIZUVRKBMN-UHFFFAOYSA-N
Formula:	C8H7ClOS
SMILES:	Cc1ccc(OC(=S)Cl)cc1
Mol. weight [g/mol]:	186.66
CAS:	937-63-3

Physical Properties

Property code	Value	Unit	Source
gf	119.39	kJ/mol	Joback Method
hf	15.15	kJ/mol	Joback Method
hfus	20.12	kJ/mol	Joback Method
hvap	49.86	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.898		Crippen Method
mcvol	129.980	ml/mol	McGowan Method
pc	3754.57	kPa	Joback Method
tb	543.99	K	Joback Method
tc	788.39	K	Joback Method
tf	305.28	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.28	J/mol×K	543.99	Joback Method
cpg	261.66	J/mol×K	584.72	Joback Method
cpg	271.25	J/mol×K	625.46	Joback Method
cpg	280.10	J/mol×K	666.19	Joback Method
cpg	288.26	J/mol×K	706.92	Joback Method

cpg	295.80	J/mol×K	747.66	Joback Method
cpg	302.77	J/mol×K	788.39	Joback Method

Sources

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=C937633&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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