O-4-Methylphenyl chlorothioformate

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

Physical Properties

Property code	Value	Unit	Source
hfus	20.12	kJ/mol	Joback Method
ie	8.22	eV	Cheméo Relay (1.0)
logp	2.898		Crippen Method
mcvol	129.980	ml/mol	McGowan Method
tb	490.73	K	Cheméo Relay (1.0)
tc	733.09	K	Cheméo Relay (1.0)
tf	255.22	K	Cheméo Relay (1.0)

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C937633&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point