(Phenylthio)acetyl chloride

Inchi: InChI=1S/C8H7ClOS/c9-8(10)6-11-7-4-2-1-3-5-7/h1-5H,6H2
InchiKey: TWOLQIUHVMTAAE-UHFFFAOYSA-N
Formula: C8H7ClOS
SMILES: O=C(Cl)CSc1ccccc1
Mol. weight [g/mol]: 186.66
CAS: 7031-27-8

Physical Properties

Property code	Value	Unit	Source
gf	21.16	kJ/mol	Joback Method
hf	-58.37	kJ/mol	Joback Method
hfus	20.44	kJ/mol	Joback Method
hvap	53.63	kJ/mol	Joback Method
log10ws	-2.56		Crippen Method
logp	2.544		Crippen Method
mcvol	129.980	ml/mol	McGowan Method
pc	3848.31	kPa	Joback Method
rinpol	1416.00		NIST Webbook
tb	569.20	K	Joback Method
tc	818.08	K	Joback Method
tf	320.59	K	Joback Method
vc	0.484	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.32	J/mol×K	569.20	Joback Method
cpg	271.39	J/mol×K	610.68	Joback Method
cpg	281.58	J/mol×K	652.16	Joback Method
cpg	290.93	J/mol×K	693.64	Joback Method
cpg	299.48	J/mol×K	735.12	Joback Method
cpg	307.26	J/mol×K	776.60	Joback Method
cpg	314.30	J/mol×K	818.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7031278&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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