1-(p-Chlorophenylthio)-2-propanol

Inchi: InChI=1S/C9H11ClOS/c1-7(11)6-12-9-4-2-8(10)3-5-9/h2-5,7,11H,6H2,1H3
InchiKey: CHHYHUZLMAKWAS-UHFFFAOYSA-N
Formula: C9H11ClOS
SMILES: CC(O)CSc1ccc(Cl)cc1
Mol. weight [g/mol]: 202.70
CAS: 13663-04-2

Physical Properties

Property code	Value	Unit	Source
gf	9.61	kJ/mol	Joback Method
hf	-135.41	kJ/mol	Joback Method
hfus	21.61	kJ/mol	Joback Method
hvap	66.06	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.813		Crippen Method
mcvol	148.370	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
tb	634.93	K	Joback Method
tc	856.77	K	Joback Method
tf	340.27	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.13	J/mol×K	634.93	Joback Method
cpg	348.98	J/mol×K	671.90	Joback Method
cpg	359.09	J/mol×K	708.88	Joback Method
cpg	368.49	J/mol×K	745.85	Joback Method
cpg	377.22	J/mol×K	782.83	Joback Method
cpg	385.29	J/mol×K	819.80	Joback Method
cpg	392.74	J/mol×K	856.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13663042&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume