Rhodanine, 5-p-chlorobenzylidene

Inchi: InChI=1S/C10H6ClNOS2/c11-7-3-1-6(2-4-7)5-8-9(13)12-10(14)15-8/h1-5H,(H,12,13,14)/
InchiKey: HIWUQEXWRIIIKB-VMPITWQZSA-N
Formula: C10H6ClNOS2
SMILES: OC1=NC(=S)SC1=Cc1ccc(Cl)cc1
Mol. weight [g/mol]: 255.74
CAS: 6318-37-2

Physical Properties

Property code	Value	Unit	Source
gf	344.89	kJ/mol	Joback Method
hf	241.85	kJ/mol	Joback Method
hfus	32.44	kJ/mol	Joback Method
hvap	83.66	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.669		Crippen Method
mcvol	165.030	ml/mol	McGowan Method
pc	4534.68	kPa	Joback Method
tb	794.37	K	Joback Method
tc	1059.11	K	Joback Method
tf	589.58	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.15	J/mol×K	794.37	Joback Method
cpg	396.53	J/mol×K	838.49	Joback Method
cpg	404.18	J/mol×K	882.62	Joback Method
cpg	411.19	J/mol×K	926.74	Joback Method
cpg	417.66	J/mol×K	970.86	Joback Method
cpg	423.67	J/mol×K	1014.99	Joback Method
cpg	429.32	J/mol×K	1059.11	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=C6318372&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