2-(4-Chlorophenyl)-2-oxoethyl ethyldithiocarbamate

Inchi: InChI=1S/C11H12ClNOS2/c1-2-13-11(15)16-7-10(14)8-3-5-9(12)6-4-8/h3-6H,2,7H2,1H3
InchiKey: SNMCUPFPILSLNS-UHFFFAOYSA-N
Formula: C11H12ClNOS2
SMILES: CCNC(=S)SCC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 273.80
CAS: 116401-18-4

Physical Properties

Property code	Value	Unit	Source
gf	243.24	kJ/mol	Joback Method
hf	68.21	kJ/mol	Joback Method
hfus	37.53	kJ/mol	Joback Method
hvap	74.13	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.150		Crippen Method
mcvol	194.280	ml/mol	McGowan Method
pc	3052.41	kPa	Joback Method
tb	763.03	K	Joback Method
tc	1015.45	K	Joback Method
tf	453.85	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.14	J/mol×K	763.03	Joback Method
cpg	480.16	J/mol×K	805.10	Joback Method
cpg	490.27	J/mol×K	847.17	Joback Method
cpg	499.58	J/mol×K	889.24	Joback Method
cpg	508.18	J/mol×K	931.31	Joback Method
cpg	516.16	J/mol×K	973.38	Joback Method
cpg	523.61	J/mol×K	1015.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116401184&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