2-Propenethioamide, 3-(4-chlorophenyl)-2-cyano-, (E)-

Inchi: InChI=1S/C10H7ClN2S/c11-9-3-1-7(2-4-9)5-8(6-12)10(13)14/h1-5H,(H2,13,14)/b8-5+

InchiKey: RZHHDALLVIGWBS-VMPITWQZSA-N

Formula: C10H7ClN2S

SMILES: N#CC(=Cc1ccc(Cl)cc1)C(N)=S

Mol. weight [g/mol]: 222.69

CAS: 68029-53-8

Physical Properties

Property code	Value	Unit	Source
gf	512.53	kJ/mol	Joback Method
hf	412.19	kJ/mol	Joback Method
hfus	29.70	kJ/mol	Joback Method
hvap	73.06	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	2.533		Crippen Method
mcvol	159.350	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
tb	745.98	K	Joback Method
tc	1016.91	K	Joback Method
tf	434.80	K	Joback Method
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.92	J/mol×K	745.98	Joback Method
cpg	365.34	J/mol×K	791.14	Joback Method
cpg	373.12	J/mol×K	836.29	Joback Method
cpg	380.43	J/mol×K	881.45	Joback Method
cpg	387.40	J/mol×K	926.60	Joback Method
cpg	394.20	J/mol×K	971.76	Joback Method
cpg	400.99	J/mol×K	1016.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68029538&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