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

Inchi: InChI=1S/C10H7N3O2S/c11-6-8(10(12)16)5-7-1-3-9(4-2-7)13(14)15/h1-5H,(H2,12,16)/b8

InchiKey: ZJUPLUDEWMWRRF-VMPITWQZSA-N

Formula: C10H7N3O2S

SMILES: N#CC(=Cc1ccc([N+](=O)[O-])cc1)C(N)=S

Mol. weight [g/mol]: 233.25

CAS: 68029-55-0

Physical Properties

Property code	Value	Unit	Source
gf	560.01	kJ/mol	Joback Method
hf	417.17	kJ/mol	Joback Method
hfus	36.87	kJ/mol	Joback Method
hvap	85.27	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	1.788		Crippen Method
mcvol	164.530	ml/mol	McGowan Method
pc	3589.94	kPa	Joback Method
tb	860.39	K	Joback Method
tc	1144.70	K	Joback Method
tf	548.49	K	Joback Method
vc	0.641	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.25	J/mol×K	860.39	Joback Method
cpg	421.43	J/mol×K	907.78	Joback Method
cpg	429.22	J/mol×K	955.16	Joback Method
cpg	436.81	J/mol×K	1002.55	Joback Method
cpg	444.37	J/mol×K	1049.93	Joback Method
cpg	452.10	J/mol×K	1097.32	Joback Method
cpg	460.17	J/mol×K	1144.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C68029550&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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