2-Propenethioamide, 2-cyano-3-(3-methoxyphenyl)-

Inchi: InChI=1S/C11H10N2OS/c1-14-10-4-2-8(3-5-10)6-9(7-12)11(13)15/h2-6H,1H3,(H2,13,15)
InchiKey: NSDYZWFBGUGNTC-RMKNXTFCSA-N
Formula: C11H10N2OS
SMILES: COc1ccc(C=C(C#N)C(=N)S)cc1
Mol. weight [g/mol]: 218.28
CAS: 137451-60-6

Physical Properties

Property code	Value	Unit	Source
gf	477.36	kJ/mol	Joback Method
hf	331.59	kJ/mol	Joback Method
hvap	74.76	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	2.509		Crippen Method
mcvol	167.070	ml/mol	McGowan Method
tb	758.48	K	Joback Method
tf	426.09	K	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.56	J/mol×K	758.48	Joback Method
cpg	83.08	J/mol×K	100.12	Joback Method
cpg	83.08	J/mol×K	100.12	Joback Method
cpg	83.08	J/mol×K	100.12	Joback Method
cpg	83.08	J/mol×K	100.12	Joback Method
cpg	83.08	J/mol×K	100.12	Joback Method
cpg	83.08	J/mol×K	100.12	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C137451606&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation 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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point