

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

Inchi:	InChI=1S/C10H7FN2S/c11-9-3-1-7(2-4-9)5-8(6-12)10(13)14/h1-5H,(H2,13,14)/b8-5+
InchiKey:	TXTBVZMAVKCLRA-VMPITWQZSA-N
Formula:	C10H7FN2S
SMILES:	N#CC(=Cc1ccc(F)cc1)C(N)=S
Mol. weight [g/mol]:	206.24
CAS:	68029-40-3

Physical Properties

Property code	Value	Unit	Source
gf	329.65	kJ/mol	Joback Method
hf	231.82	kJ/mol	Joback Method
hfus	28.59	kJ/mol	Joback Method
hvap	67.86	kJ/mol	Joback Method
log10ws	-3.62		Crippen Method
logp	2.019		Crippen Method
mcvol	148.880	ml/mol	McGowan Method
pc	3356.75	kPa	Joback Method
tb	707.82	K	Joback Method
tc	964.44	K	Joback Method
tf	405.47	K	Joback Method
vc	0.578	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.74	J/molxK	707.82	Joback Method
cpg	355.59	J/molxK	750.59	Joback Method
cpg	363.72	J/molxK	793.36	Joback Method
cpg	371.29	J/molxK	836.13	Joback Method
cpg	378.40	J/molxK	878.90	Joback Method
cpg	385.19	J/molxK	921.67	Joback Method
cpg	391.80	J/molxK	964.44	Joback Method

Sources

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=C68029403&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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