Propiolamide

Other names:	HC«equiv»CCONH2
	2-Propynamide
	Propynamide
Inchi:	InChI=1S/C3H3NO/c1-2-3(4)5/h1H,(H2,4,5)
InchiKey:	HCJTYESURSHXNB-UHFFFAOYSA-N
Formula:	C3H3NO
SMILES:	C#CC(N)=O
Mol. weight [g/mol]:	69.06
CAS:	7341-96-0

Physical Properties

Property code	Value	Unit	Source
gf	134.98	kJ/mol	Joback Method
hf	107.86	kJ/mol	Joback Method
hfus	13.30	kJ/mol	Joback Method
hvap	39.52	kJ/mol	Joback Method
ie	9.85	eV	NIST Webbook
ie	10.50	eV	NIST Webbook
log10ws	-0.08		Crippen Method
logp	-0.895		Crippen Method
mcvol	56.080	ml/mol	McGowan Method
pc	6524.67	kPa	Joback Method
tb	384.56	K	Joback Method
tc	596.99	K	Joback Method
tf	303.73	K	Joback Method
vc	0.201	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	94.66	J/mol×K	384.56	Joback Method
cpg	98.98	J/mol×K	419.96	Joback Method
cpg	103.03	J/mol×K	455.37	Joback Method
cpg	106.84	J/mol×K	490.77	Joback Method

cpg	110.41	J/mol×K	526.18	Joback Method
cpg	113.75	J/mol×K	561.58	Joback Method
cpg	116.89	J/mol×K	596.99	Joback Method

Sources

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=C7341960&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
ie:	Ionization energy
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