Oct-2-ynamide

Inchi: InChI=1S/C8H13NO/c1-2-3-4-5-6-7-8(9)10/h2-5H2,1H3,(H2,9,10)
InchiKey: OCHGSVAVCZKJBA-UHFFFAOYSA-N
Formula: C8H13NO
SMILES: CCCCCC#CC(N)=O
Mol. weight [g/mol]: 139.19
CAS: 117821-02-0

Physical Properties

Property code	Value	Unit	Source
chs	-4817.90	kJ/mol	NIST Webbook
gf	156.81	kJ/mol	Joback Method
hf	-14.94	kJ/mol	Joback Method
hfl	-188.10 ± 4.00	kJ/mol	NIST Webbook
hfs	230.00	kJ/mol	NIST Webbook
hfus	26.39	kJ/mol	Joback Method
hvap	52.94	kJ/mol	Joback Method
log10ws	-2.18		Crippen Method
logp	1.055		Crippen Method
mcvol	126.530	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
tb	517.84	K	Joback Method
tc	729.14	K	Joback Method
tf	419.21	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.32	J/mol×K	517.84	Joback Method
cpg	291.14	J/mol×K	553.06	Joback Method
cpg	302.37	J/mol×K	588.27	Joback Method
cpg	313.02	J/mol×K	623.49	Joback Method
cpg	323.13	J/mol×K	658.71	Joback Method
cpg	332.70	J/mol×K	693.93	Joback Method

cpg	341.76	J/mol×K	729.14	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=C117821020&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfs:	Solid phase 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