

Oxanamide

Inchi:	InChI=1S/C8H15NO2/c1-3-5-6-8(4-2,11-6)7(9)10/h6H,3-5H2,1-2H3,(H2,9,10)
InchiKey:	WBLPIVIXQOFTPQ-UHFFFAOYSA-N
Formula:	C8H15NO2
SMILES:	CCCC1OC1(CC)C(N)=O
Mol. weight [g/mol]:	157.21
CAS:	126-93-2

Physical Properties

Property code	Value	Unit	Source
gf	-84.56	kJ/mol	Joback Method
hf	-351.54	kJ/mol	Joback Method
hfus	24.16	kJ/mol	Joback Method
hvap	53.75	kJ/mol	Joback Method
log10ws	-1.59		Crippen Method
logp	0.819		Crippen Method
mcvol	130.140	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
rinpol	1249.00		NIST Webbook
tb	538.10	K	Joback Method
tc	746.05	K	Joback Method
tf	377.28	K	Joback Method
vc	0.493	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.52	J/molxK	538.10	Joback Method
cpg	342.71	J/molxK	572.76	Joback Method
cpg	355.05	J/molxK	607.42	Joback Method
cpg	366.66	J/molxK	642.08	Joback Method
cpg	377.64	J/molxK	676.73	Joback Method
cpg	388.11	J/molxK	711.39	Joback Method
cpg	398.18	J/molxK	746.05	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=C126932&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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