Acetic acid, [2-[(2-propenylamino)carbonyl]phenoxy]-

Other names: Acetic acid, (o-(allylcarbamoyl)phenoxy)-
Acetic acid, (o-(N-allylcarbamoyl)phenoxy)-
Benzamide, N-allyl-, o-(carboxymethoxy)-
[2-[(allylamino)carbonyl]phenoxy]acetic acid

Inchi: InChI=1S/C12H13NO4/c1-2-7-13-12(16)9-5-3-4-6-10(9)17-8-11(14)15/h2-6H,1,7-8H2,(H

InchiKey: IHBWXJXQXPFUAE-UHFFFAOYSA-N

Formula: C12H13NO4

SMILES: C=CCNC(=O)c1ccccc1OCC(=O)O

Mol. weight [g/mol]: 235.24

CAS: 119-45-9

Physical Properties

Property code	Value	Unit	Source
gf	-169.49	kJ/mol	Joback Method
hf	-396.66	kJ/mol	Joback Method
hfus	32.78	kJ/mol	Joback Method
hvap	83.59	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.066		Crippen Method
mcvol	176.740	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
tb	774.81	K	Joback Method
tc	980.36	K	Joback Method
tf	497.75	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.16	J/mol×K	774.81	Joback Method
cpg	497.20	J/mol×K	809.07	Joback Method
cpg	506.51	J/mol×K	843.33	Joback Method
cpg	515.12	J/mol×K	877.58	Joback Method
cpg	523.04	J/mol×K	911.84	Joback Method

cpg	530.30	J/mol×K	946.10	Joback Method
cpg	536.92	J/mol×K	980.36	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=C119459&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
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