

Acetic acid, oxo(phenylamino)-

Other names:	Oxanilic acid N-Phenyloxamic acid Oxamic acid, phenyl- Kyselina oxalanilova 2-Phenylamino-2-oxoacetic acid
Inchi:	InChI=1S/C8H7NO3/c10-7(8(11)12)9-6-4-2-1-3-5-6/h1-5H,(H,9,10)(H,11,12)
InchiKey:	PQJZHMCWDKOPQG-UHFFFAOYSA-N
Formula:	C8H7NO3
SMILES:	O=C(O)C(=O)Nc1ccccc1
Mol. weight [g/mol]:	165.15
CAS:	500-72-1

Physical Properties

Property code	Value	Unit	Source
gf	-176.38	kJ/mol	Joback Method
hf	-295.84	kJ/mol	Joback Method
hfus	22.90	kJ/mol	Joback Method
hvap	72.28	kJ/mol	Joback Method
log10ws	-0.77		Crippen Method
logp	0.710		Crippen Method
mcvol	118.810	ml/mol	McGowan Method
pc	4931.51	kPa	Joback Method
tb	659.21	K	Joback Method
tc	872.55	K	Joback Method
tf	419.68	K	Joback Method
vc	0.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.32	J/mol×K	659.21	Joback Method
cpg	297.76	J/mol×K	694.77	Joback Method
cpg	305.55	J/mol×K	730.32	Joback Method
cpg	312.74	J/mol×K	765.88	Joback Method

cpg	319.36	J/mol×K	801.43	Joback Method
cpg	325.43	J/mol×K	836.99	Joback Method
cpg	330.99	J/mol×K	872.55	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=C500721&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
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

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