

3-Morpholinone, 5-methyl-6-phenyl-

Other names:	Fenmetramide Feninetramide McN-1075 5-Methyl-6-phenyl-3-morpholinone
Inchi:	InChI=1S/C11H13NO2/c1-8-11(14-7-10(13)12-8)9-5-3-2-4-6-9/h2-6,8,11H,7H2,1H3,(H,1
InchiKey:	UJEPHPADGSWWRM-UHFFFAOYSA-N
Formula:	C11H13NO2
SMILES:	CC1N=C(O)COC1c1ccccc1
Mol. weight [g/mol]:	191.23
CAS:	5588-29-4

Physical Properties

Property code	Value	Unit	Source
gf	85.06	kJ/mol	Joback Method
hf	-166.81	kJ/mol	Joback Method
hfus	29.23	kJ/mol	Joback Method
hvap	70.83	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	2.103		Crippen Method
mcvol	148.650	ml/mol	McGowan Method
pc	3602.88	kPa	Joback Method
tb	669.61	K	Joback Method
tc	901.44	K	Joback Method
tf	415.50	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.06	J/molxK	669.61	Joback Method
cpg	438.54	J/molxK	708.25	Joback Method
cpg	452.85	J/molxK	746.89	Joback Method
cpg	466.00	J/molxK	785.53	Joback Method
cpg	478.00	J/molxK	824.16	Joback Method

cpg	488.86	J/mol×K	862.80	Joback Method
cpg	498.61	J/mol×K	901.44	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=C5588294&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
hvac:	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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