

Phenoxypropazine

Inchi:	InChI=1S/C9H14N2O/c1-8(11-10)7-12-9-5-3-2-4-6-9/h2-6,8,11H,7,10H2,1H3
InchiKey:	QNEXFJFTGQBXBJ-UHFFFAOYSA-N
Formula:	C9H14N2O
SMILES:	CC(COc1ccccc1)NN
Mol. weight [g/mol]:	166.22
CAS:	3818-37-9

Physical Properties

Property code	Value	Unit	Source
gf	185.71	kJ/mol	Joback Method
hf	-42.80	kJ/mol	Joback Method
hfus	21.07	kJ/mol	Joback Method
hvap	57.00	kJ/mol	Joback Method
log10ws	-2.15		Crippen Method
logp	0.917		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
rinpol	1468.00		NIST Webbook
rinpol	1468.00		NIST Webbook
tb	576.68	K	Joback Method
tc	798.25	K	Joback Method
tf	360.76	K	Joback Method
vc	0.507	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.03	J/molxK	576.68	Joback Method
cpg	357.11	J/molxK	613.61	Joback Method
cpg	370.30	J/molxK	650.54	Joback Method
cpg	382.66	J/molxK	687.46	Joback Method
cpg	394.19	J/molxK	724.39	Joback Method
cpg	404.93	J/molxK	761.32	Joback Method
cpg	414.90	J/molxK	798.25	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3818379&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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