

PROPAFENONE-H2O, M(HO-)-H2O, AC

Inchi:	InChI=1S/C23H25NO3/c1-3-16-24(19(2)25)17-9-18-27-23-13-8-7-12-21(23)22(26)15-14
InchiKey:	FQTQILLIEHGPAT-ITWXKMDCSA-N
Formula:	C23H25NO3
SMILES:	CCCN(CC=COc1cccc1C(=O)C=Cc1cccc1)C(C)=O
Mol. weight [g/mol]:	363.45

Physical Properties

Property code	Value	Unit	Source
gf	266.35	kJ/mol	Joback Method
hf	-111.87	kJ/mol	Joback Method
hfus	50.83	kJ/mol	Joback Method
hvap	89.87	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	4.734		Crippen Method
mcvol	297.800	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
tb	934.90	K	Joback Method
tc	1164.98	K	Joback Method
tf	558.73	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	914.98	J/molxK	934.90	Joback Method
cpg	929.62	J/molxK	973.25	Joback Method
cpg	943.26	J/molxK	1011.59	Joback Method
cpg	956.02	J/molxK	1049.94	Joback Method
cpg	968.03	J/molxK	1088.29	Joback Method
cpg	979.39	J/molxK	1126.63	Joback Method
cpg	990.22	J/molxK	1164.98	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=R255380&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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