Propafenone

Other names:	Rhytmol
	1-Propanone, 1-[2-[2-hydroxy-3-(propylamino)propoxy]phenyl]-3-phenyl-
	1-(2-(2-Hydroxy-3-(propylamino)propoxy)phenyl)-3-phenyl-1-propanone
	2'-[2-Hydroxy-3-(propylamino)propoxy]-3-phenylpropiophenone
Inchi:	InChI=1S/C21H27NO3/c1-2-14-22-15-18(23)16-25-21-11-7-6-10-19(21)20(24)13-12-17-8
InchiKey:	JWHAUXFOSRPERK-UHFFFAOYSA-N
Formula:	C21H27NO3
SMILES:	CCCNCC(O)COc1ccccc1C(=O)CCc1ccccc1
Mol. weight [g/mol]:	341.44
CAS:	54063-53-5

Physical Properties

Property code	Value	Unit	Source
gf	57.34	kJ/mol	Joback Method
hf	-364.02	kJ/mol	Joback Method
hfus	46.29	kJ/mol	Joback Method
hvap	99.44	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	3.241		Crippen Method
mcvol	282.520	ml/mol	McGowan Method
pc	1696.30	kPa	Joback Method
tb	956.42	K	Joback Method
tc	1176.74	K	Joback Method
tf	562.43	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	910.85	J/mol×K	956.42	Joback Method
cpg	923.94	J/mol×K	993.14	Joback Method
cpg	935.94	J/mol×K	1029.86	Joback Method
cpg	946.90	J/mol×K	1066.58	Joback Method
cpg	956.88	J/mol×K	1103.30	Joback Method

cpg	965.96	J/mol×K	1140.02	Joback Method
cpg	974.20	J/mol×K	1176.74	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=C54063535&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