Propoxyphene M (des-Ac, dehydro)

Inchi: InChI=1S/C19H23N/c1-16(15-20(2)3)19(18-12-8-5-9-13-18)14-17-10-6-4-7-11-17/h4-13H

InchiKey: SUSOPMJVIJKACW-KNTRCKAVSA-N

Formula: C19H23N

SMILES: CC(CN(C)C)=C(Cc1ccccc1)c1ccccc1

Mol. weight [g/mol]: 265.39

Physical Properties

Property code	Value	Unit	Source
gf	507.82	kJ/mol	Joback Method
hf	202.74	kJ/mol	Joback Method
hfus	33.65	kJ/mol	Joback Method
hvap	64.60	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	4.264		Crippen Method
mcvol	236.730	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	1678.00		NIST Webbook
rinpol	1678.00		NIST Webbook
tb	703.84	K	Joback Method
tc	934.03	K	Joback Method
tf	356.20	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.58	J/mol×K	703.84	Joback Method
cpg	669.12	J/mol×K	742.20	Joback Method
cpg	687.24	J/mol×K	780.57	Joback Method
cpg	704.06	J/mol×K	818.93	Joback Method
cpg	719.68	J/mol×K	857.30	Joback Method
cpg	734.24	J/mol×K	895.66	Joback Method
cpg	747.86	J/mol×K	934.03	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R311316&Units=SI

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