Dextropropoxyphene 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/h4-14,
InchiKey: DXPIDNMXZDVKHC-RGEXLXHISA-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	513.93	kJ/mol	Joback Method
hf	207.25	kJ/mol	Joback Method
hfus	31.44	kJ/mol	Joback Method
hvap	64.13	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.425		Crippen Method
mcvol	236.730	ml/mol	McGowan Method
pc	1862.72	kPa	Joback Method
rinpol	1687.00		NIST Webbook
tb	703.52	K	Joback Method
tc	934.42	K	Joback Method
tf	355.16	K	Joback Method
vc	0.876	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.39	J/mol×K	703.52	Joback Method
cpg	670.05	J/mol×K	742.00	Joback Method
cpg	688.25	J/mol×K	780.49	Joback Method
cpg	705.13	J/mol×K	818.97	Joback Method
cpg	720.78	J/mol×K	857.45	Joback Method
cpg	735.35	J/mol×K	895.93	Joback Method
cpg	748.95	J/mol×K	934.42	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=R307887&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