Dothiepin

Other names:	1-Propanamine, 3-dibenzo[b,e]thiepin-11(6H)-ylidene-N,N-dimethyl- Dosulepin Dibenzo[b,e]thiepin, 1-propanamine deriv. Dibenzo[b,e]thiepin-«DELTA»11(6H),«gamma»-propylamine, N,N-dimethyl- Dosulepine IZ 914 Prothiaden Prothiadene Propylamine, N,N-dimethyl-3-(dibenzo(b,e)thiepin-«DELTA»(11(6H),«gamma»)- 3-Dibenzo(b,e)thiepin-11(6H)-ylidene-N,N-dimethyl-1-propamine 11-(3-Dimethylaminopropylidene)-6,11-dihydrodibenzo(b,e)thiepin N,N-Dimethyldibenzo(b,e)thiepin-«DELTA»11(6H,«gamma»-propylamine Prothiaden spofa 3-Dibenzo[b,e]thiepin-11(6H)-ylidine-N,N-dimethyl-propanamine Dothep
Inchi:	InChI=1S/C19H21NS/c1-20(2)13-7-11-17-16-9-4-3-8-15(16)14-21-19-12-6-5-10-18(17)19
InchiKey:	PHTUQLWOUWZIMZ-GZTJUZNOSA-N
Formula:	C19H21NS
SMILES:	CN(C)CCC=C1c2ccccc2CSc2ccccc21
Mol. weight [g/mol]:	295.44
CAS:	113-53-1

Physical Properties

Property code	Value	Unit	Source
gf	579.22	kJ/mol	Joback Method
hf	296.59	kJ/mol	Joback Method
hfus	36.33	kJ/mol	Joback Method
hvap	72.63	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.676		Crippen Method
mcvol	242.220	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinpol	2385.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook
rinpol	2364.00		NIST Webbook
rinpol	2385.00		NIST Webbook

rinpol	2364.00		NIST Webbook
rinpol	2460.50		NIST Webbook
rinpol	2380.00		NIST Webbook
tb	775.76	K	Joback Method
tc	1020.33	K	Joback Method
tf	530.23	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.66	J/mol×K	775.76	Joback Method
cpg	694.86	J/mol×K	816.52	Joback Method
cpg	710.87	J/mol×K	857.28	Joback Method
cpg	725.85	J/mol×K	898.04	Joback Method
cpg	739.97	J/mol×K	938.80	Joback Method
cpg	753.38	J/mol×K	979.57	Joback Method
cpg	766.24	J/mol×K	1020.33	Joback Method

Sources

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=C113531&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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