Doxepin

Other names: 1-Propanamine, 3-dibenz[b,e]oxepin-11(6H)-ylidene-N,N-dimethyl-
11-(3-Dimethylaminopropylidene)-6,11-dihydrodibenz(b,e)oxipin
3-Dibenz[b,e]oxepin-11(6H)-ylidene-N,N-dimethyl-1-propanamine
Dibenz(b,e)oxepin-«delta»11(6H),«gamma»-propylamine, N,N-dimethyl-
Dibenz(b,e)oxepin-Â«deltaÂ»11(6H),Â«gammaÂ»-propylamine, N,N-dimethyl-
Doxepine
N,N-Dimethyldibenz(b,e)oxepin-«delta»11(6H),«gamma»-propylamine
N,N-Dimethyldibenz(b,e)oxepin-Â«deltaÂ»11(6H),Â«gammaÂ»-propylamine
NSC 108160

Inchi: InChI=1S/C19H21NO/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: ODQWQRRAPPTVAG-BOPFTXTBSA-N

Formula: C19H21NO

SMILES: CN(C)CCC=C1c2ccccc2COc2ccccc21

Mol. weight [g/mol]: 279.38

CAS: 1668-19-5

Physical Properties

Property code	Value	Unit	Source
gf	453.24	kJ/mol	Joback Method
hf	119.33	kJ/mol	Joback Method
hfus	40.66	kJ/mol	Joback Method
hvap	71.33	kJ/mol	Joback Method
log10ws	-3.40		Aqueous Solubility Prediction Method
logp	3.962		Crippen Method
mcvol	231.740	ml/mol	McGowan Method
pc	2012.70	kPa	Joback Method
rinpol	2226.00		NIST Webbook
rinpol	2194.00		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2217.00		NIST Webbook
rinpol	2196.00		NIST Webbook
rinpol	2220.00		NIST Webbook
rinpol	2215.00		NIST Webbook
rinpol	2242.00		NIST Webbook
rinpol	2217.00		NIST Webbook
rinpol	2210.00		NIST Webbook

rinpol	2242.00		NIST Webbook
rinpol	2217.00		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2231.00		NIST Webbook
rinpol	2226.00		NIST Webbook
rinpol	2239.00		NIST Webbook
rinpol	2235.00		NIST Webbook
tb	754.88	K	Joback Method
tc	988.07	K	Joback Method
tf	473.35	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.75	J/mol×K	754.88	Joback Method
cpg	678.87	J/mol×K	793.74	Joback Method
cpg	694.81	J/mol×K	832.61	Joback Method
cpg	709.69	J/mol×K	871.47	Joback Method
cpg	723.66	J/mol×K	910.34	Joback Method
cpg	736.83	J/mol×K	949.20	Joback Method
cpg	749.34	J/mol×K	988.07	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1668195&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