Orphenadrine

Other names:	Norflex
	Ethanamine, N,N-dimethyl-2-[(2-methylphenyl)phenylmethoxy]-
	o-Methyldiphenhydramine
	Brocadisipal
	Disipal
	Orphenadrin
	Orphenedrine
	Phenyl-o-tolylmethyl dimethylaminoethyl ether
	WS 2434
	2-Methyldiphenhydramine
	Ethylamine, N,N-dimethyl-2-((o-methyl-«alpha»-phenylbenzyl)oxy)-
	«beta»-Dimethylaminoethyl 2-methylbenzhydryl ether
	Biorphen
	BS-5930
	N,N-Dimethyl-2-[(o-methyl-«alpha»-phenylbenzyl)oxy]ethylamine
	ORP
	Orphenadine
Inchi:	InChI=1S/C18H23NO/c1-15-9-7-8-12-17(15)18(20-14-13-19(2)3)16-10-5-4-6-11-16/h4-12
InchiKey:	QVYRGXJJSLMXQH-UHFFFAOYSA-N
Formula:	C18H23NO
SMILES:	Cc1ccccc1C(OCCN(C)C)c1ccccc1
Mol. weight [g/mol]:	269.38
CAS:	83-98-7

Physical Properties

Property code	Value	Unit	Source
gf	319.21	kJ/mol	Joback Method
hf	-23.23	kJ/mol	Joback Method
hfus	30.75	kJ/mol	Joback Method
hvap	64.94	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.663		Crippen Method
mcvol	232.810	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
rinpol	1924.00		NIST Webbook
rinpol	1932.00		NIST Webbook
rinpol	1943.00		NIST Webbook

rinpol	1932.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1927.00		NIST Webbook
rinpol	1950.00		NIST Webbook
rinpol	1924.00		NIST Webbook
rinpol	1924.00		NIST Webbook
rinpol	1943.00		NIST Webbook
rinpol	1925.00		NIST Webbook
rinpol	1924.00		NIST Webbook
rinpol	1915.00		NIST Webbook
rinpol	1924.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1940.00		NIST Webbook
rinpol	1924.00		NIST Webbook
rinpol	1925.00		NIST Webbook
rinpol	1936.00		NIST Webbook
rinpol	1915.00		NIST Webbook
ripol	2562.00		NIST Webbook
ripol	2562.00		NIST Webbook
tb	704.00	K	Joback Method
tc	924.74	K	Joback Method
tf	397.68	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.71	J/mol×K	704.00	Joback Method
cpg	665.59	J/mol×K	740.79	Joback Method
cpg	683.16	J/mol×K	777.58	Joback Method
cpg	699.47	J/mol×K	814.37	Joback Method
cpg	714.60	J/mol×K	851.16	Joback Method
cpg	728.60	J/mol×K	887.95	Joback Method
cpg	741.53	J/mol×K	924.74	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=C83987&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume