Methylphenidate

Other names:	Concerta
	2-Piperidineacetic acid, «alpha»-phenyl-, methyl ester
	«alpha»-Phenyl-2-piperidineacetic acid methyl ester
	Calocain
	Meridil
	Methyl «alpha»-phenyl-«alpha»-(2-piperidyl)acetate
	Methyl phenidyl acetate
	Methylphenidan
	Phenidylate
	4311/b Ciba
	NCI-C56280
	Plimasine
	Methyl «alpha»-phenyl-«alpha»-2-piperidinylacetate
	Methyl «alpha»-phenyl-2-piperidine-acetate
	Rubifen
	Ritalin
	Centedein
	Centredin
	Ritaline
	Ritcher works
	Methyl phenyl(2-piperidinyl)acetate
Inchi:	InChI=1S/C14H19NO2/c1-17-14(16)13(11-7-3-2-4-8-11)12-9-5-6-10-15-12/h2-4,7-8,12-1
InchiKey:	DUGOZIWVEXMGBE-UHFFFAOYSA-N
Formula:	C14H19NO2
SMILES:	COC(=O)C(c1ccccc1)C1CCCCN1
Mol. weight [g/mol]:	233.31
CAS:	113-45-1

Physical Properties

Property code	Value	Unit	Source
gf	55.21	kJ/mol	Joback Method
hf	-253.71	kJ/mol	Joback Method
hfus	26.75	kJ/mol	Joback Method
hvap	64.99	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.085		Crippen Method

mcvol	190.920	ml/mol	McGowan Method
pc	2637.96	kPa	Joback Method
rinpol	1763.60		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1753.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1763.60		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1695.00		NIST Webbook
rinpol	1704.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1737.00		NIST Webbook
rinpol	1742.00		NIST Webbook
rinpol	1737.00		NIST Webbook
ripol	2385.00		NIST Webbook
ripol	2385.00		NIST Webbook
tb	690.35	K	Joback Method
tc	932.60	K	Joback Method
tf	443.53	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	535.99	J/mol×K	690.35	Joback Method
cpg	555.28	J/mol×K	730.72	Joback Method
cpg	573.06	J/mol×K	771.10	Joback Method
cpg	589.39	J/mol×K	811.47	Joback Method
cpg	604.30	J/mol×K	851.85	Joback Method
cpg	617.83	J/mol×K	892.22	Joback Method
cpg	630.00	J/mol×K	932.60	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=C113451&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