Methadone

Other names:	3-Heptanone, 6-(dimethylamino)-4,4-diphenyl-
	Adanon
	Algovetin
	Amidon
	Amidone
	Diaminon
	Dolophin
	Heptadone
	Ketalgin
	Phenadone
	Physeptone
	Dolophine
	Heptanon
	Methadon
	3-Heptanone, 6-(dimethylamino)-4,4-diphenyl-, (.+/-.)-
	(.+/-.)-Methadone
	dl-Methadone
	Racemic methadone
	2-Dimethylamino-4,4-diphenyl-5-heptanone
	6-(Dimethylamino)-4,4-diphenyl-3-heptanone
	Heptanon (pharmaceutical)
	Sedo-Rapide
	Methadone M
Inchi:	InChI=1S/C21H27NO/c1-5-20(23)21(16-17(2)22(3)4,18-12-8-6-9-13-18)19-14-10-7-11-15
InchiKey:	USSIQXCVUWKGNF-UHFFFAOYSA-N
Formula:	C21H27NO
SMILES:	CCC(=O)C(CC(C)N(C)C)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	309.45
CAS:	76-99-3

Physical Properties

Property code	Value	Unit	Source
gf	333.02	kJ/mol	Joback Method
hf	-62.79	kJ/mol	Joback Method
hfus	31.91	kJ/mol	Joback Method
hvap	74.00	kJ/mol	Joback Method

log10ws	-4.56		Crippen Method
logp	4.292		Crippen Method
mcvol	270.780	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
rinpol	2141.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2137.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2170.00		NIST Webbook
rinpol	2170.00		NIST Webbook
rinpol	2182.10		NIST Webbook
rinpol	2141.00		NIST Webbook
rinpol	2109.00		NIST Webbook
rinpol	2131.00		NIST Webbook
rinpol	2135.00		NIST Webbook
rinpol	2185.00		NIST Webbook
rinpol	2131.00		NIST Webbook
rinpol	2139.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2137.00		NIST Webbook
rinpol	2121.00		NIST Webbook
rinpol	2121.00		NIST Webbook
rinpol	2131.00		NIST Webbook
rinpol	2135.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2137.00		NIST Webbook
rinpol	2136.00		NIST Webbook
rinpol	2170.00		NIST Webbook
rinpol	2148.00		NIST Webbook
rinpol	2139.00		NIST Webbook
rinpol	2182.10		NIST Webbook
rinpol	2185.00		NIST Webbook
rinpol	2121.00		NIST Webbook
rinpol	2150.00		NIST Webbook
tb	795.88	K	Joback Method
tc	1024.40	K	Joback Method
tf	449.09	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	810.86	J/mol×K	795.88	Joback Method
cpg	829.20	J/mol×K	833.97	Joback Method
cpg	846.17	J/mol×K	872.05	Joback Method
cpg	861.88	J/mol×K	910.14	Joback Method
cpg	876.47	J/mol×K	948.22	Joback Method
cpg	890.07	J/mol×K	986.31	Joback Method
cpg	902.81	J/mol×K	1024.40	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C76993&Units=SI
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

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