

Isomethadone

Other names:	3-Hexanone, 6-(dimethylamino)-4,4-diphenyl-5-methyl- 6-Dimethylamino-5-methyl-4,4-diphenyl-3-hexanone 1,1-Diphenyl-1-(dimethylaminoisopropyl)butanone-2 Isoamidone ii Isomethadone ii Isadanone Isoamidone Liden (I-form) Win-1783
Inchi:	InChI=1S/C21H27NO/c1-5-20(23)21(17(2)16-22(3)4,18-12-8-6-9-13-18)19-14-10-7-11-1
InchiKey:	IFKPLJWIEQBPGG-UHFFFAOYSA-N
Formula:	C21H27NO
SMILES:	CCC(=O)C(c1ccccc1)(c1ccccc1)C(C)CN(C)C
Mol. weight [g/mol]:	309.45
CAS:	466-40-0

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	-4.20		Crippen Method
logp	4.149		Crippen Method
mcvol	270.780	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
rinsol	2128.00		NIST Webbook
tb	795.88	K	Joback Method
tc	1024.40	K	Joback Method
tf	449.09	K	Joback Method
vc	1.002	m ³ /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

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=C466400&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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

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