Normethadone

Other names:	3-Hexanone, 6-(dimethylamino)-4,4-diphenyl-
	Dacartil
	Desmethylmethadone
	Eucopon
	Hoechst 10582
	Isoamidone I
	Isomethadone I
	Mepidon
	Noramidone
	Normedon
	Phenyldimazone
	6-Dimethylamino-4,4-diphenyl-3-hexanone
	6-Dimethylamio-4-diphenyl-3-hexanone
	NSC 19598
	1-Dimethylamino-3,3-diphenyl-4-hexanone
Inchi:	InChI=1S/C20H25NO/c1-4-19(22)20(15-16-21(2)3,17-11-7-5-8-12-17)18-13-9-6-10-14-18
InchiKey:	WCJFBSYALHQBSK-UHFFFAOYSA-N
Formula:	C20H25NO
SMILES:	CCC(=O)C(CCN(C)C)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	295.42
CAS:	467-85-6

Physical Properties

Property code	Value	Unit	Source
gf	327.04	kJ/mol	Joback Method
hf	-36.87	kJ/mol	Joback Method
hfus	32.84	kJ/mol	Joback Method
hvap	72.16	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.904		Crippen Method
mcvol	256.690	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
rinpol	2095.00		NIST Webbook
rinpol	2091.00		NIST Webbook
rinpol	2090.00		NIST Webbook
rinpol	2095.00		NIST Webbook
tb	773.44	K	Joback Method

tc	1001.66	K	Joback Method
tf	452.82	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	753.07	J/mol×K	773.44	Joback Method
cpg	771.08	J/mol×K	811.48	Joback Method
cpg	787.72	J/mol×K	849.51	Joback Method
cpg	803.13	J/mol×K	887.55	Joback Method
cpg	817.41	J/mol×K	925.59	Joback Method
cpg	830.71	J/mol×K	963.62	Joback Method
cpg	843.14	J/mol×K	1001.66	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C467856&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