Noracymethadol

Other names:	Benzeneethanol, «alpha»-ethyl-«beta»-[2-(methylamino)propyl]-«beta»-phenyl-, acetate (ester) 3-Heptanol, 6-(methylamino)-4,4-diphenyl-, acetate (ester) Noracetylmethadol Noracetylmethadone Normethadyl acetate Benzeneethanol, «alpha»-ethyl-«beta»-[2-(methylamino)propyl]-«beta»-phenyl-, acetate 6-(Methylamino)-4,4-diphenyl-3-heptanol acetate (ester) 3-Heptanol, 6-(methylamino)-4,4-diphenyl-, acetate 5633-25-0
Inchi:	InChI=1S/C22H29NO2/c1-5-21(25-18(3)24)22(16-17(2)23-4,19-12-8-6-9-13-19)20-14-10
InchiKey:	VWCUGCYZZGRKEE-UHFFFAOYSA-N
Formula:	C22H29NO2
SMILES:	CCC(OC(C)=O)C(CC(C)NC)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	339.47
CAS:	1477-39-0

Physical Properties

Property code	Value	Unit	Source
gf	212.61	kJ/mol	Joback Method
hf	-234.99	kJ/mol	Joback Method
hfus	34.24	kJ/mol	Joback Method
hvap	82.64	kJ/mol	Joback Method
log10ws	-5.29		Crippen Method
logp	4.312		Crippen Method
mcvol	290.740	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
tb	878.47	K	Joback Method
tc	1107.61	K	Joback Method
tf	487.78	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	915.44	J/mol×K	878.47	Joback Method
cpg	932.18	J/mol×K	916.66	Joback Method
cpg	947.58	J/mol×K	954.85	Joback Method
cpg	961.77	J/mol×K	993.04	Joback Method
cpg	974.84	J/mol×K	1031.23	Joback Method
cpg	986.91	J/mol×K	1069.42	Joback Method
cpg	998.08	J/mol×K	1107.61	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1477390&Units=SI

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

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume