1,1-DIPHENYL-4-PIPERIDINO-1-BUTANOL

Other names: 1-Piperidinebutanol, «alpha»,«alpha»-diphenyl-
Benzhydrol, «alpha»-(3-piperidinopropyl)-
Difenidol
«alpha»,«alpha»-Diphenyl-1-piperidinebutanol
Nometic
SKF 478
SK&F 478
Vontrol
Avomol
Cephadol
Diphenyl(3-(1-piperidyl)propyl)carbinol

Inchi: InChI=1S/C21H27NO/c23-21(19-11-4-1-5-12-19,20-13-6-2-7-14-20)15-10-18-22-16-8-3-9

InchiKey: OGAKLTJNUQRZJU-UHFFFAOYSA-N

Formula: C21H27NO

SMILES: OC(CCCN1CCCCC1)(c1ccccc1)c1ccccc1

Mol. weight [g/mol]: 309.45

Physical Properties

Property code	Value	Unit	Source
hf	-43.83	kJ/mol	Cheméo Relay (1.0)
hvap	110.31	kJ/mol	Cheméo Relay (1.0)
log10ws	-2.66		Cheméo Relay (1.0)
logp	4.189		Crippen Method
mcvol	264.220	ml/mol	McGowan Method
rinpol	2390.00		NIST Webbook
rinpol	2384.00		NIST Webbook
rinpol	2384.00		NIST Webbook
rinpol	2384.00		NIST Webbook
tb	659.88	K	Cheméo Relay (1.0)
tf	381.30	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C972021&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

hf:	Enthalpy of formation 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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point