Alphamethadol

Other names:	Benzeneethanol, «beta»-[2-(dimethylamino)propyl]-«alpha»-ethyl-«beta»-phenyl-, [R-(R*,R*)]- 3-Heptanol, 6-(dimethylamino)-4,4-diphenyl-, (3R,6R)-(+)- «alpha»-Methadol «alpha»-Methadol, (+)- Alphamethadol, (+)- (3R,6R)-6-Dimethylamino-4,4-diphenyl-3-heptanol
Inchi:	InChI=1S/C21H29NO/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:	QIRAYNIFEOXSPW-UHFFFAOYSA-N
Formula:	C21H29NO
SMILES:	CCC(O)C(CC(C)N(C)C)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	311.46
CAS:	17199-54-1

Physical Properties

Property code	Value	Unit	Source
gf	322.68	kJ/mol	Joback Method
hf	-107.72	kJ/mol	Joback Method
hfus	30.88	kJ/mol	Joback Method
hvap	83.54	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.084		Crippen Method
mcvol	275.080	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
tb	833.75	K	Joback Method
tc	1048.56	K	Joback Method
tf	444.98	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.24	J/mol×K	833.75	Joback Method

cpg	872.90	J/mol×K	869.55	Joback Method
cpg	888.43	J/mol×K	905.35	Joback Method
cpg	902.96	J/mol×K	941.15	Joback Method
cpg	916.59	J/mol×K	976.96	Joback Method
cpg	929.42	J/mol×K	1012.76	Joback Method
cpg	941.59	J/mol×K	1048.56	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=C17199541&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume