Alphacetylmethadol

Other names: Acetylmethadol
Inchi: InChI=1S/C23H31NO2/c1-6-22(26-19(3)25)23(17-18(2)24(4)5,20-13-9-7-10-14-20)21-15
InchiKey: XBMIVRRWGCYBTQ-UHFFFAOYSA-N
Formula: C23H31NO2
SMILES: CCC(OC(C)=O)C(CC(C)N(C)C)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]: 353.50
CAS: 17199-58-5

Physical Properties

Property code	Value	Unit	Source
gf	242.42	kJ/mol	Joback Method
hf	-241.57	kJ/mol	Joback Method
hfus	34.76	kJ/mol	Joback Method
hvap	80.47	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.655		Crippen Method
mcvol	304.830	ml/mol	McGowan Method
pc	1387.11	kPa	Joback Method
rinpol	2187.00		NIST Webbook
rinpol	2187.00		NIST Webbook
tb	863.62	K	Joback Method
tc	1088.26	K	Joback Method
tf	478.86	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	958.11	J/mol×K	863.62	Joback Method
cpg	975.97	J/mol×K	901.06	Joback Method
cpg	992.48	J/mol×K	938.50	Joback Method
cpg	1007.75	J/mol×K	975.94	Joback Method
cpg	1021.89	J/mol×K	1013.38	Joback Method
cpg	1035.01	J/mol×K	1050.82	Joback Method

cpg	1047.23	J/mol×K	1088.26	Joback Method

Sources

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=C17199585&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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