Ketocaine

Inchi: InChI=1S/C18H29NO2/c1-6-9-17(20)16-10-7-8-11-18(16)21-13-12-19(14(2)3)15(4)5/h7-8
InchiKey: UXAWFWFJXIANHZ-UHFFFAOYSA-N
Formula: C18H29NO2
SMILES: CCCC(=O)c1ccccc1OCCN(C(C)C)C(C)C
Mol. weight [g/mol]: 291.43
CAS: 1092-46-2

Physical Properties

Property code	Value	Unit	Source
gf	75.44	kJ/mol	Joback Method
hf	-377.62	kJ/mol	Joback Method
hfus	34.79	kJ/mol	Joback Method
hvap	69.02	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.167		Crippen Method
mcvol	258.140	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	2019.00		NIST Webbook
tb	730.75	K	Joback Method
tc	927.66	K	Joback Method
tf	406.19	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.95	J/mol×K	730.75	Joback Method
cpg	771.23	J/mol×K	763.57	Joback Method
cpg	788.42	J/mol×K	796.39	Joback Method
cpg	804.56	J/mol×K	829.20	Joback Method
cpg	819.68	J/mol×K	862.02	Joback Method
cpg	833.83	J/mol×K	894.84	Joback Method
cpg	847.04	J/mol×K	927.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1092462&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