Ketobisnortilidine

Inchi: InChI=1S/C15H17NO3/c1-2-19-14(18)15(11-6-4-3-5-7-11)10-12(17)8-9-13(15)16/h3-9,13
InchiKey: OTRJPTAJPGIPRO-UHFFFAOYSA-N
Formula: C15H17NO3
SMILES: CCOC(=O)C1(c2ccccc2)CC(=O)C=CC1N
Mol. weight [g/mol]: 259.30

Physical Properties

Property code	Value	Unit	Source
gf	-61.02	kJ/mol	Joback Method
hf	-358.11	kJ/mol	Joback Method
hfus	23.97	kJ/mol	Joback Method
hvap	74.56	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	1.344		Crippen Method
mcvol	202.280	ml/mol	McGowan Method
pc	2668.02	kPa	Joback Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tb	800.20	K	Joback Method
tc	1056.62	K	Joback Method
tf	536.67	K	Joback Method
vc	0.744	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.71	J/mol×K	800.20	Joback Method
cpg	628.07	J/mol×K	842.94	Joback Method
cpg	644.51	J/mol×K	885.67	Joback Method
cpg	660.17	J/mol×K	928.41	Joback Method
cpg	675.19	J/mol×K	971.15	Joback Method
cpg	689.73	J/mol×K	1013.89	Joback Method
cpg	703.92	J/mol×K	1056.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R18030&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