Bornaprine

Inchi: InChI=1S/C21H31NO2/c1-3-22(4-2)13-8-14-24-20(23)21(18-9-6-5-7-10-18)16-17-11-12-
InchiKey: BDNMABJZSXTKAQ-UHFFFAOYSA-N
Formula: C21H31NO2
SMILES: CCN(CC)CCCOC(=O)C1(c2ccccc2)CC2CCC1C2
Mol. weight [g/mol]: 329.48
CAS: 20448-86-6

Physical Properties

Property code	Value	Unit	Source
gf	211.41	kJ/mol	Joback Method
hf	-283.17	kJ/mol	Joback Method
hfus	38.94	kJ/mol	Joback Method
hvap	74.35	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	4.020		Crippen Method
mcvol	278.690	ml/mol	McGowan Method
pc	1523.50	kPa	Joback Method
rinpol	2255.00		NIST Webbook
rinpol	2255.00		NIST Webbook
tb	808.61	K	Joback Method
tc	1023.76	K	Joback Method
tf	509.50	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	899.51	J/mol×K	808.61	Joback Method
cpg	920.44	J/mol×K	844.47	Joback Method
cpg	940.63	J/mol×K	880.33	Joback Method
cpg	960.26	J/mol×K	916.18	Joback Method
cpg	979.51	J/mol×K	952.04	Joback Method
cpg	998.58	J/mol×K	987.90	Joback Method
cpg	1017.65	J/mol×K	1023.76	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=C20448866&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