Bamipine, N-desalkyl, hydroxy, acetylated

Inchi: InChI=1S/C17H17NO3/c1-13(19)18(12-15-6-4-3-5-7-15)16-8-10-17(11-9-16)21-14(2)20/h
InchiKey: WICIDZZWMSJMKS-UHFFFAOYSA-N
Formula: C17H17NO3
SMILES: CC(=O)Oc1ccc(N(Cc2ccccc2)C(C)=O)cc1
Mol. weight [g/mol]: 283.32

Physical Properties

Property code	Value	Unit	Source
gf	55.39	kJ/mol	Joback Method
hf	-222.47	kJ/mol	Joback Method
hfus	34.89	kJ/mol	Joback Method
hvap	76.59	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.165		Crippen Method
mcvol	221.860	ml/mol	McGowan Method
pc	2276.24	kPa	Joback Method
rinpol	2340.00		NIST Webbook
rinpol	2340.00		NIST Webbook
tb	789.30	K	Joback Method
tc	1020.92	K	Joback Method
tf	501.27	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.63	J/mol×K	789.30	Joback Method
cpg	640.95	J/mol×K	827.90	Joback Method
cpg	654.06	J/mol×K	866.51	Joback Method
cpg	666.00	J/mol×K	905.11	Joback Method
cpg	676.86	J/mol×K	943.71	Joback Method
cpg	686.68	J/mol×K	982.32	Joback Method
cpg	695.53	J/mol×K	1020.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R536060&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

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