Bamipine, N-desalkyl, acetylated

Inchi: InChI=1S/C15H15NO/c1-13(17)16(15-10-6-3-7-11-15)12-14-8-4-2-5-9-14/h2-11H,12H2,1
InchiKey: BISSQVWYQNHTIH-UHFFFAOYSA-N
Formula: C15H15NO
SMILES: CC(=O)N(Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 225.29
CAS: 6840-29-5

Physical Properties

Property code	Value	Unit	Source
gf	282.10	kJ/mol	Joback Method
hf	75.08	kJ/mol	Joback Method
hfus	27.31	kJ/mol	Joback Method
hvap	62.33	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.240		Crippen Method
mcvol	186.240	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	2080.00		NIST Webbook
rinpol	2080.00		NIST Webbook
tb	662.27	K	Joback Method
tc	899.64	K	Joback Method
tf	394.05	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.02	J/mol×K	662.27	Joback Method
cpg	495.53	J/mol×K	701.83	Joback Method
cpg	510.70	J/mol×K	741.39	Joback Method
cpg	524.62	J/mol×K	780.95	Joback Method
cpg	537.37	J/mol×K	820.52	Joback Method
cpg	549.06	J/mol×K	860.08	Joback Method
cpg	559.78	J/mol×K	899.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6840295&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