Axillaridine

Inchi: InChI=1S/C30H42N2O2/c1-19(32(4)5)22-13-14-23-21-11-12-25-27(33)26(31-28(34)20-9
InchiKey: ZMAOKPMWBVUQPK-NMWVCJJNSA-N
Formula: C30H42N2O2
SMILES: CC(C1CCC2C3CCC4C(=O)C(NC(=O)c5ccccc5)=CCC4(C)C3CCC21C)N(C)C
Mol. weight [g/mol]: 462.67

Physical Properties

Property code	Value	Unit	Source
gf	429.07	kJ/mol	Joback Method
hf	-284.39	kJ/mol	Joback Method
hfus	46.69	kJ/mol	Joback Method
hvap	101.97	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	5.698		Crippen Method
mcvol	385.160	ml/mol	McGowan Method
pc	1116.31	kPa	Joback Method
rinpol	2418.00		NIST Webbook
rinpol	2416.00		NIST Webbook
rinpol	2403.00		NIST Webbook
tb	1135.26	K	Joback Method
tc	1397.24	K	Joback Method
tf	745.08	K	Joback Method
vc	1.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1554.97	J/mol×K	1135.26	Joback Method
cpg	1595.28	J/mol×K	1178.92	Joback Method
cpg	1638.08	J/mol×K	1222.59	Joback Method
cpg	1683.88	J/mol×K	1266.25	Joback Method
cpg	1733.20	J/mol×K	1309.91	Joback Method
cpg	1786.56	J/mol×K	1353.58	Joback Method
cpg	1844.46	J/mol×K	1397.24	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=R178119&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