

APRINDINE, M(HO-), AC

Inchi:	InChI=1S/C24H32N2O2/c1-4-25(5-2)14-9-15-26(22-10-7-6-8-11-22)23-16-20-12-13-24(2
InchiKey:	ZBKVUDHLNABUKM-UHFFFAOYSA-N
Formula:	C24H32N2O2
SMILES:	CCN(CC)CCCN(c1ccccc1)C1Cc2ccc(OC(C)=O)cc2C1
Mol. weight [g/mol]:	380.52

Physical Properties

Property code	Value	Unit	Source
gf	405.15	kJ/mol	Joback Method
hf	-125.51	kJ/mol	Joback Method
hfus	52.18	kJ/mol	Joback Method
hvap	88.05	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.318		Crippen Method
mcvol	318.040	ml/mol	McGowan Method
pc	1353.63	kPa	Joback Method
rinsol	2850.00		NIST Webbook
tb	919.75	K	Joback Method
tc	1140.59	K	Joback Method
tf	593.16	K	Joback Method
vc	1.181	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.38	J/mol×K	919.75	Joback Method
cpg	1058.70	J/mol×K	956.56	Joback Method
cpg	1074.89	J/mol×K	993.36	Joback Method
cpg	1090.06	J/mol×K	1030.17	Joback Method
cpg	1104.32	J/mol×K	1066.98	Joback Method
cpg	1117.80	J/mol×K	1103.78	Joback Method
cpg	1130.61	J/mol×K	1140.59	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=R255028&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
mccvol:	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

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