APRINDINE, M (DESPHENYL-), AC

Inchi: InChI=1S/C19H29NO/c1-4-16(5-2)9-8-12-20(15(3)21)19-13-17-10-6-7-11-18(17)14-19/h
InchiKey: KNJRAWJGBHUARB-UHFFFAOYSA-N
Formula: C19H29NO
SMILES: CCC(CC)CCCN(C(C)=O)C1Cc2ccccc2C1
Mol. weight [g/mol]: 287.44

Physical Properties

Property code	Value	Unit	Source
gf	252.05	kJ/mol	Joback Method
hf	-187.96	kJ/mol	Joback Method
hfus	37.85	kJ/mol	Joback Method
hvap	69.14	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.219		Crippen Method
mcvol	255.500	ml/mol	McGowan Method
pc	1565.99	kPa	Joback Method
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
tb	738.39	K	Joback Method
tc	941.68	K	Joback Method
tf	428.17	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.73	J/mol×K	738.39	Joback Method
cpg	783.67	J/mol×K	772.27	Joback Method
cpg	801.47	J/mol×K	806.15	Joback Method
cpg	818.21	J/mol×K	840.04	Joback Method
cpg	833.97	J/mol×K	873.92	Joback Method
cpg	848.82	J/mol×K	907.80	Joback Method
cpg	862.85	J/mol×K	941.68	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=R255013&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