

APRINDINE, M (DESINDANE-), AC

Inchi:	InChI=1S/C16H25NO/c1-4-15(5-2)10-9-13-17(14(3)18)16-11-7-6-8-12-16/h6-8,11-12,15
InchiKey:	ZENIDPFCJVWVNQ-UHFFFAOYSA-N
Formula:	C16H25NO
SMILES:	CCC(CC)CCCN(C(C)=O)c1ccccc1
Mol. weight [g/mol]:	247.38

Physical Properties

Property code	Value	Unit	Source
gf	175.67	kJ/mol	Joback Method
hf	-187.37	kJ/mol	Joback Method
hfus	32.33	kJ/mol	Joback Method
hvap	61.89	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	4.256		Crippen Method
mcvol	224.090	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	1880.00		NIST Webbook
rinpol	1880.00		NIST Webbook
tb	658.03	K	Joback Method
tc	855.92	K	Joback Method
tf	363.90	K	Joback Method
vc	0.842	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.37	J/mol×K	658.03	Joback Method
cpg	629.48	J/mol×K	691.01	Joback Method
cpg	646.51	J/mol×K	723.99	Joback Method
cpg	662.53	J/mol×K	756.97	Joback Method
cpg	677.57	J/mol×K	789.95	Joback Method
cpg	691.69	J/mol×K	822.94	Joback Method
cpg	704.94	J/mol×K	855.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=R255008&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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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