

APRINDINE, M(N-DESALKYL-)

Inchi:	InChI=1S/C15H15N/c1-2-8-14(9-3-1)16-15-10-12-6-4-5-7-13(12)11-15/h1-9,15-16H,10-1
InchiKey:	MHVHCDLCLNXADJ-UHFFFAOYSA-N
Formula:	C15H15N
SMILES:	<chem>c1ccc(NC2Cc3ccccc3C2)cc1</chem>
Mol. weight [g/mol]:	209.29

Physical Properties

Property code	Value	Unit	Source
gf	440.75	kJ/mol	Joback Method
hf	234.93	kJ/mol	Joback Method
hfus	25.53	kJ/mol	Joback Method
hvap	60.55	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.266		Crippen Method
mvol	173.810	ml/mol	McGowan Method
pc	2865.80	kPa	Joback Method
rinpol	1920.00		NIST Webbook
rinpol	1920.00		NIST Webbook
tb	657.85	K	Joback Method
tc	908.22	K	Joback Method
tf	394.77	K	Joback Method
vc	0.651	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.84	J/mol×K	657.85	Joback Method
cpg	477.52	J/mol×K	699.58	Joback Method
cpg	493.74	J/mol×K	741.31	Joback Method
cpg	508.63	J/mol×K	783.03	Joback Method
cpg	522.33	J/mol×K	824.76	Joback Method
cpg	534.95	J/mol×K	866.49	Joback Method
cpg	546.65	J/mol×K	908.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R255033&Units=SI
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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