

p-Dimethylaminobenzylidene-p-isopropylphenylamine

Inchi:	InChI=1S/C20H22N2/c1-15(2)17-7-9-18(10-8-17)19(14-21)13-16-5-11-20(12-6-16)22(3)4
InchiKey:	NGFFOQFGBWGLU-CPNJWEJPSA-N
Formula:	C20H22N2
SMILES:	CC(C)c1ccc(C(C#N)=Cc2ccc(N(C)C)cc2)cc1
Mol. weight [g/mol]:	290.40
CAS:	53407-79-7

Physical Properties

Property code	Value	Unit	Source
chs	-11083.00	kJ/mol	NIST Webbook
gf	636.27	kJ/mol	Joback Method
hf	328.55	kJ/mol	Joback Method
hfs	68.58	kJ/mol	NIST Webbook
hfus	34.76	kJ/mol	Joback Method
hvap	78.16	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.940		Crippen Method
mcvol	252.200	ml/mol	McGowan Method
pc	1641.76	kPa	Joback Method
tb	838.44	K	Joback Method
tc	1077.04	K	Joback Method
tf	456.46	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.86	J/molxK	838.44	Joback Method
cpg	750.56	J/molxK	878.21	Joback Method
cpg	765.15	J/molxK	917.97	Joback Method
cpg	778.74	J/molxK	957.74	Joback Method
cpg	791.44	J/molxK	997.51	Joback Method
cpg	803.38	J/molxK	1037.27	Joback Method
cpg	814.66	J/molxK	1077.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53407797&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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