

4-(4-amino-3,5-dimethylphenyl)-2,6-dimethylaniline

Inchi:	InChI=1S/C16H20N2/c1-9-5-13(6-10(2)15(9)17)14-7-11(3)16(18)12(4)8-14/h5-8H,17-18H
InchiKey:	UAIUNKRWKOVEES-UHFFFAOYSA-N
Formula:	C16H20N2
SMILES:	Cc1cc(-c2cc(C)c(N)c(C)c2)cc(C)c1N
Mol. weight [g/mol]:	240.35
CAS:	54827-17-7

Physical Properties

Property code	Value	Unit	Source
af	0.7355		Cheméo Relay (1.0)
hfus	33.34	kJ/mol	Joback Method
hvap	115.11	kJ/mol	Cheméo Relay (1.0)
ie	7.01	eV	Cheméo Relay (1.0)
logp	3.752		Crippen Method
mcvol	208.740	ml/mol	McGowan Method
pc	2338.29	kPa	Joback Method
tb	639.80	K	Cheméo Relay (1.0)
tc	931.45	K	Cheméo Relay (1.0)
tf	457.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	1.93100e+01
Coeff. B	1.13288e+00
Coeff. C	-5.93560e-04
Coeff. D	1.02800e-07
Coeff. E	0.00000e+00
Basis	predicted

Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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

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