

2,3,4,5,6-pentamethylaniline

Inchi:	InChI=1S/C11H17N/c1-6-7(2)9(4)11(12)10(5)8(6)3/h12H2,1-5H3
InchiKey:	DCBKKCYNUSINPI-UHFFFAOYSA-N
Formula:	C11H17N
SMILES:	Cc1c(C)c(C)c(N)c(C)c1C
Mol. weight [g/mol]:	163.26
CAS:	2243-30-3

Physical Properties

Property code	Value	Unit	Source
af	0.5306		Cheméo Relay (1.0)
hf	-41.67	kJ/mol	Cheméo Relay (1.0)
hfus	21.54	kJ/mol	Joback Method
hvap	73.55	kJ/mol	Cheméo Relay (1.0)
ie	7.16	eV	Cheméo Relay (1.0)
log10ws	-2.89		Cheméo Relay (1.0)
logp	2.811		Crippen Method
mcvol	152.070	ml/mol	McGowan Method
pc	2600.43	kPa	Joback Method
tb	544.42	K	Cheméo Relay (1.0)
tc	780.32	K	Cheméo Relay (1.0)
tf	407.82	K	Cheméo Relay (1.0)
vc	0.548	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.54	J/mol×K	575.19	Joback Method
cpg	375.86	J/mol×K	611.43	Joback Method
cpg	389.52	J/mol×K	647.67	Joback Method
cpg	402.51	J/mol×K	683.92	Joback Method
cpg	414.84	J/mol×K	720.16	Joback Method
cpg	426.54	J/mol×K	756.40	Joback Method
cpg	437.59	J/mol×K	792.64	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52740e+01
Coeff. B	-4.66384e+03
Coeff. C	-8.84900e+01
Temperature range (K), min.	399.69
Temperature range (K), max.	556.63

Sources

The Yaws Handbook of Vapor Pressure:
Joback Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
https://en.wikipedia.org/wiki/Joback_method

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):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
pvap: Vapor pressure

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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