

o-Toluidine, 5-isopropyl-

Other names:	2-Amino-p-cymene 2-Cymidine 2-Methyl-5-isopropylaniline 5-Isopropyl-2-methylaniline 5-Isopropyl-2-methylphenylamine 5-Isopropyl-o-toluidine Aniline, 5-isopropyl-2-methyl- Benzenamine, 2-methyl-5-(1-methylethyl)- Carvacrylamine p-Cymen-2-amine p-Cymene, 2-amino-
Inchi:	InChI=1S/C10H15N/c1-7(2)9-5-4-8(3)10(11)6-9/h4-7H,11H2,1-3H3
InchiKey:	YKWALWNGEXPARQ-UHFFFAOYSA-N
Formula:	C10H15N
SMILES:	<chem>Cc1ccc(C(C)C)cc1N</chem>
Mol. weight [g/mol]:	149.23
CAS:	2051-53-8

Physical Properties

Property code	Value	Unit	Source
gf	190.48	kJ/mol	Joback Method
hf	-7.63	kJ/mol	Joback Method
hfus	16.59	kJ/mol	Joback Method
hvap	51.71	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.701		Crippen Method
mcvol	137.980	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
tb	536.93	K	Joback Method
tc	759.90	K	Joback Method
tf	322.18	K	Joback Method
vc	0.510	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	381.82	J/molxK	722.74	Joback Method
cpg	316.41	J/molxK	536.93	Joback Method
cpg	331.10	J/molxK	574.09	Joback Method
cpg	344.96	J/molxK	611.25	Joback Method
cpg	358.01	J/molxK	648.41	Joback Method
cpg	370.29	J/molxK	685.57	Joback Method
cpg	392.63	J/molxK	759.90	Joback Method
hvapt	72.00	kJ/mol	373.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49469e+01
Coeff. B	-4.43707e+03
Coeff. C	-8.43200e+01
Temperature range (K), min.	387.00
Temperature range (K), max.	544.82

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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=C2051538&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvac:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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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