

2,2,2-Trifluoro-N-methyl-N-(1-phenylpropan-2-yl)aniline

Inchi:	InChI=1S/C12H14F3NO/c1-9(8-10-6-4-3-5-7-10)16(2)11(17)12(13,14)15/h3-7,9H,8H2,1H3
InchiKey:	AXAFMXNUGNZMCK-UHFFFAOYSA-N
Formula:	C12H14F3NO
SMILES:	CC(Cc1ccccc1)N(C)C(=O)C(F)(F)F
Mol. weight [g/mol]:	245.24

Physical Properties

Property code	Value	Unit	Source
af	0.4571		Cheméo Relay (1.0)
hf	-755.06	kJ/mol	Cheméo Relay (1.0)
hfus	23.80	kJ/mol	Joback Method
hvap	69.80	kJ/mol	Cheméo Relay (1.0)
ie	8.99	eV	Cheméo Relay (1.0)
log10ws	-1.50		Cheméo Relay (1.0)
logp	2.638		Crippen Method
mcvol	173.040	ml/mol	McGowan Method
pc	2298.11	kPa	Joback Method
rinpol	1389.00		NIST Webbook
rinpol	1389.00		NIST Webbook
tb	516.03	K	Cheméo Relay (1.0)
tc	677.99	K	Cheméo Relay (1.0)
tf	262.55	K	Cheméo Relay (1.0)
vc	0.613	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.30	J/mol×K	561.09	Joback Method
cpg	447.46	J/mol×K	593.17	Joback Method
cpg	461.60	J/mol×K	625.26	Joback Method
cpg	474.78	J/mol×K	657.34	Joback Method
cpg	487.06	J/mol×K	689.43	Joback Method
cpg	498.49	J/mol×K	721.51	Joback Method
cpg	509.13	J/mol×K	753.59	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U412214&Units=SI>

Joback Method: 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

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

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