

m-Toluic acid hydrazide

Other names:	3-Toluic hydrazide Benzoic acid, 3-methyl-, hydrazide m-Toluic acid hydrazide m-Toluic hydrazide m-toluohydrazide
Inchi:	InChI=1S/C8H10N2O/c1-6-3-2-4-7(5-6)8(11)10-9/h2-5H,9H2,1H3,(H,10,11)
InchiKey:	XFNNAMBYJSQXKF-UHFFFAOYSA-N
Formula:	C8H10N2O
SMILES:	Cc1cccc(C(=O)NN)c1
Mol. weight [g/mol]:	150.18

Physical Properties

Property code	Value	Unit	Source
af	0.5515		Cheméo Relay (1.0)
gf	146.18	kJ/mol	Joback Method
hf	-35.34	kJ/mol	Cheméo Relay (1.0)
hfus	22.02	kJ/mol	Joback Method
hvap	76.54	kJ/mol	Cheméo Relay (1.0)
ie	8.91	eV	Cheméo Relay (1.0)
log10ws	-1.46		Cheméo Relay (1.0)
logp	0.599		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
tb	568.94	K	Cheméo Relay (1.0)
tc	812.34	K	Cheméo Relay (1.0)
tf	341.36	K	Cheméo Relay (1.0)
vc	0.431	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	286.50	J/mol×K	590.67	Joback Method
cpg	297.98	J/mol×K	629.44	Joback Method
cpg	308.67	J/mol×K	668.21	Joback Method

cpg	318.60	J/mol×K	706.98	Joback Method
cpg	327.79	J/mol×K	745.75	Joback Method
cpg	336.28	J/mol×K	784.52	Joback Method
cpg	344.12	J/mol×K	823.28	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C13050470&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

Cheméo Relay (1.0):

Legend

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

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