

«alpha»,«alpha»,«alpha»-Trifluoro-m-formotoluidide

Other names:	3'-Trifluoromethylformanilide Formamide, N-[3-(trifluoromethyl)phenyl]- m-Formotoluidide, «alpha»,«alpha»,«alpha»-trifluoro- Formanilide, 3'-trifluoromethyl- N-(3-Trifluoromethylphenyl)formamide N-(«alpha»,«alpha»,«alpha»-Trifluoro-m-tolyl)formamide
Inchi:	InChI=1S/C8H6F3NO/c9-8(10,11)6-2-1-3-7(4-6)12-5-13/h1-5H,(H,12,13)
InchiKey:	PPECHNDWLRNHEA-UHFFFAOYSA-N
Formula:	C8H6F3NO
SMILES:	O=CNc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	189.13
CAS:	657-78-3

Physical Properties

Property code	Value	Unit	Source
gf	-472.46	kJ/mol	Joback Method
hf	-612.58	kJ/mol	Joback Method
hfus	19.34	kJ/mol	Joback Method
hvap	45.75	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.274		Crippen Method
mcvol	116.680	ml/mol	McGowan Method
pc	3464.28	kPa	Joback Method
tb	507.51	K	Joback Method
tc	706.45	K	Joback Method
tf	317.71	K	Joback Method
vc	0.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.32	J/mol×K	507.51	Joback Method
cpg	274.87	J/mol×K	540.67	Joback Method
cpg	284.66	J/mol×K	573.82	Joback Method

cpg	293.74	J/mol×K	606.98	Joback Method
cpg	302.15	J/mol×K	640.13	Joback Method
cpg	309.91	J/mol×K	673.29	Joback Method
cpg	317.08	J/mol×K	706.45	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C657783&Units=SI
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

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
hvap:	Enthalpy of vaporization at standard conditions
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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