M-toluic acid, 4-(trifluoroacetamido)-

Inchi: InChI=1S/C10H8F3NO3/c1-5-4-6(8(15)16)2-3-7(5)14-9(17)10(11,12)13/h2-4H,1H3,(H,14
InchiKey: DMBNKOMLHPNNJZ-UHFFFAOYSA-N
Formula: C10H8F3NO3
SMILES: Cc1cc(C(=O)O)ccc1NC(=O)C(F)(F)F
Mol. weight [g/mol]: 247.17

Physical Properties

Property code	Value	Unit	Source
gf	-760.39	kJ/mol	Joback Method
hf	-957.14	kJ/mol	Joback Method
hfus	29.13	kJ/mol	Joback Method
hvap	74.31	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.194		Crippen Method
mcvol	152.300	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
tb	709.51	K	Joback Method
tc	905.06	K	Joback Method
tf	471.45	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.27	J/mol×K	709.51	Joback Method
cpg	418.75	J/mol×K	742.10	Joback Method
cpg	426.60	J/mol×K	774.69	Joback Method
cpg	433.88	J/mol×K	807.29	Joback Method
cpg	440.60	J/mol×K	839.88	Joback Method
cpg	446.82	J/mol×K	872.47	Joback Method
cpg	452.56	J/mol×K	905.06	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=B6010447&Units=SI

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