3'-Trifluoromethylpropionanilide

Inchi: InChI=1S/C10H10F3NO/c1-2-9(15)14-8-5-3-4-7(6-8)10(11,12)13/h3-6H,2H2,1H3,(H,14,1
InchiKey: RQXGETUNXUENJX-UHFFFAOYSA-N
Formula: C10H10F3NO
SMILES: CCC(=O)Nc1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 217.19
CAS: 2300-88-1

Physical Properties

Property code	Value	Unit	Source
gf	-485.02	kJ/mol	Joback Method
hf	-680.86	kJ/mol	Joback Method
hfus	23.83	kJ/mol	Joback Method
hvap	50.23	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	3.054		Crippen Method
mcvol	144.860	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
tb	558.48	K	Joback Method
tc	756.68	K	Joback Method
tf	348.18	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.74	J/mol×K	558.48	Joback Method
cpg	364.17	J/mol×K	591.51	Joback Method
cpg	375.77	J/mol×K	624.55	Joback Method
cpg	386.57	J/mol×K	657.58	Joback Method
cpg	396.62	J/mol×K	690.61	Joback Method
cpg	405.96	J/mol×K	723.64	Joback Method
cpg	414.64	J/mol×K	756.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2300881&Units=SI
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

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