Glycine, N-(3-trifluoromethylbenzoyl)-, methyl ester

Inchi: InChI=1S/C11H10F3NO3/c1-18-9(16)6-15-10(17)7-3-2-4-8(5-7)11(12,13)14/h2-5H,6H2,1

InchiKey: BSCPQOKDXQXMTN-UHFFFAOYSA-N

Formula: C11H10F3NO3

SMILES: COC(=O)CNC(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 261.20

Physical Properties

Property code	Value	Unit	Source
gf	-710.52	kJ/mol	Joback Method
hf	-946.30	kJ/mol	Joback Method
hfus	29.21	kJ/mol	Joback Method
hvap	61.61	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	1.608		Crippen Method
mcvol	166.390	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	1629.00		NIST Webbook
tb	657.65	K	Joback Method
tc	858.75	K	Joback Method
tf	431.61	K	Joback Method
vc	0.651	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.83	J/mol×K	657.65	Joback Method
cpg	450.18	J/mol×K	691.17	Joback Method
cpg	460.73	J/mol×K	724.68	Joback Method
cpg	470.51	J/mol×K	758.20	Joback Method
cpg	479.56	J/mol×K	791.72	Joback Method
cpg	487.90	J/mol×K	825.24	Joback Method
cpg	495.58	J/mol×K	858.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299699&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

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