Glycine, N-(2,3,4-trifluorobenzoyl)-, methyl ester

Inchi: InChI=1S/C10H8F3NO3/c1-17-7(15)4-14-10(16)5-2-3-6(11)9(13)8(5)12/h2-3H,4H2,1H3,(

InchiKey: KEBJVTNUWUBQGP-UHFFFAOYSA-N

Formula: C10H8F3NO3

SMILES: COC(=O)CNC(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 247.17

Physical Properties

Property code	Value	Unit	Source
gf	-741.04	kJ/mol	Joback Method
hf	-939.85	kJ/mol	Joback Method
hfus	33.25	kJ/mol	Joback Method
hvap	62.00	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	1.007		Crippen Method
mcvol	152.300	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1554.00		NIST Webbook
rinpol	1554.00		NIST Webbook
tb	647.96	K	Joback Method
tc	843.40	K	Joback Method
tf	442.96	K	Joback Method
vc	0.607	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.12	J/mol×K	647.96	Joback Method
cpg	394.15	J/mol×K	680.53	Joback Method
cpg	403.60	J/mol×K	713.11	Joback Method
cpg	412.47	J/mol×K	745.68	Joback Method
cpg	420.77	J/mol×K	778.25	Joback Method
cpg	428.50	J/mol×K	810.82	Joback Method
cpg	435.66	J/mol×K	843.40	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=U299628&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume