N-(tert-Butoxycarbonyl)glycine, methyl ester

Inchi: InChI=1S/C8H15NO4/c1-8(2,3)13-7(11)9-5-6(10)12-4/h5H2,1-4H3,(H,9,11)
InchiKey: PHUZOEOLWIHIKH-UHFFFAOYSA-N
Formula: C8H15NO4
SMILES: COC(=O)CNC(=O)OC(C)(C)C
Mol. weight [g/mol]: 189.21

Physical Properties

Property code	Value	Unit	Source
gf	-359.13	kJ/mol	Joback Method
hf	-653.33	kJ/mol	Joback Method
hfus	19.74	kJ/mol	Joback Method
hvap	56.85	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	0.684		Crippen Method
mcvol	148.440	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	1274.90		NIST Webbook
tb	581.96	K	Joback Method
tc	777.53	K	Joback Method
tf	379.32	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.11	J/mol×K	581.96	Joback Method
cpg	385.48	J/mol×K	614.55	Joback Method
cpg	397.21	J/mol×K	647.15	Joback Method
cpg	408.31	J/mol×K	679.74	Joback Method
cpg	418.78	J/mol×K	712.34	Joback Method
cpg	428.64	J/mol×K	744.93	Joback Method
cpg	437.89	J/mol×K	777.53	Joback Method

Sources

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=U333189&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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