P-Hydroxyphenylacetylglycine, methyl ester

Inchi: InChI=1S/C11H13NO4/c1-16-11(15)7-12-10(14)6-8-2-4-9(13)5-3-8/h2-5,13H,6-7H2,1H3,
InchiKey: FYHWMDONXPAJDH-UHFFFAOYSA-N
Formula: C11H13NO4
SMILES: COC(=O)CNC(=O)Cc1ccc(O)cc1
Mol. weight [g/mol]: 223.23

Physical Properties

Property code	Value	Unit	Source
gf	-273.92	kJ/mol	Joback Method
hf	-515.06	kJ/mol	Joback Method
hfus	33.55	kJ/mol	Joback Method
hvap	77.71	kJ/mol	Joback Method
log10ws	-0.91		Crippen Method
logp	0.224		Crippen Method
mcvol	166.950	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
rinpol	1955.00		NIST Webbook
tb	738.71	K	Joback Method
tc	962.96	K	Joback Method
tf	526.62	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	459.03	J/mol×K	738.71	Joback Method
cpg	470.18	J/mol×K	776.09	Joback Method
cpg	480.60	J/mol×K	813.46	Joback Method
cpg	490.37	J/mol×K	850.84	Joback Method
cpg	499.55	J/mol×K	888.21	Joback Method
cpg	508.21	J/mol×K	925.59	Joback Method
cpg	516.41	J/mol×K	962.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R245660&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume