Glycine, N-benzoyl-, methyl ester

Other names:	Glycine, N-benzoyl-, methyl ester
	Methyl hippurate
	Methyl N-benzoylglycinate
	N-Benzoylglycine methyl ester
	Methyl ester of hippuric acid
	Methyl (benzoylamino)acetate
	Benzoylamino-acetic acid methyl ester
Inchi:	InChI=1S/C10H11NO3/c1-14-9(12)7-11-10(13)8-5-3-2-4-6-8/h2-6H,7H2,1H3,(H,11,13)
InchiKey:	XTKVNQKOTKPCKM-UHFFFAOYSA-N
Formula:	C10H11NO3
SMILES:	COC(=O)CNC(=O)c1ccccc1
Mol. weight [g/mol]:	193.20

Physical Properties

Property code	Value	Unit	Source
af	0.5861		Cheméo Relay (1.0)
gf	-127.72	kJ/mol	Joback Method
hf	-421.27	kJ/mol	Cheméo Relay (1.0)
hfus	25.18	kJ/mol	Joback Method
hvap	83.72	kJ/mol	Cheméo Relay (1.0)
ie	9.04	eV	Cheméo Relay (1.0)
log10ws	-2.11		Cheméo Relay (1.0)
logp	0.589		Crippen Method
mcvol	146.990	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	1722.20		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1715.40		NIST Webbook
rinpol	1720.80		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1675.00		NIST Webbook
rinpol	1675.00		NIST Webbook
tb	572.46	K	Cheméo Relay (1.0)
tc	789.04	K	Cheméo Relay (1.0)
tf	351.82	K	Cheméo Relay (1.0)
vc	0.527	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.30	J/mol×K	635.21	Joback Method
cpg	375.49	J/mol×K	671.85	Joback Method
cpg	386.85	J/mol×K	708.50	Joback Method
cpg	397.40	J/mol×K	745.14	Joback Method
cpg	407.16	J/mol×K	781.78	Joback Method
cpg	416.15	J/mol×K	818.42	Joback Method
cpg	424.40	J/mol×K	855.07	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1205089&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
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
ie: Ionization energy
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

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