(3-Phenyl-acryloylamino)-acetic acid methyl ester

Inchi: InChI=1S/C11H11NO3/c1-15-11(14)12-10(13)8-7-9-5-3-2-4-6-9/h2-8H,1H3,(H,12,13,14)/

InchiKey: KIVJMEXGGJQCFE-BQYQJAHWSA-N

Formula: C11H11NO3

SMILES: COC(=O)NC(=O)C=Cc1ccccc1

Mol. weight [g/mol]: 205.21

Physical Properties

Property code	Value	Unit	Source
gf	-39.08	kJ/mol	Joback Method
hf	-220.53	kJ/mol	Joback Method
hfus	27.97	kJ/mol	Joback Method
hvap	64.65	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	1.582		Crippen Method
mcvol	156.780	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
rinpol	2003.00		NIST Webbook
tb	662.25	K	Joback Method
tc	887.04	K	Joback Method
tf	409.82	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	390.06	J/mol×K	662.25	Joback Method
cpg	402.23	J/mol×K	699.72	Joback Method
cpg	413.51	J/mol×K	737.18	Joback Method
cpg	423.95	J/mol×K	774.65	Joback Method
cpg	433.57	J/mol×K	812.11	Joback Method
cpg	442.44	J/mol×K	849.58	Joback Method
cpg	450.58	J/mol×K	887.04	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=R247913&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