3-(phenylcarbamoyl)prop-2-enoic acid

Inchi: InChI=1S/C10H9NO3/c12-9(6-7-10(13)14)11-8-4-2-1-3-5-8/h1-7H,(H,11,12)(H,13,14)
InchiKey: WHZLCOICKHIPRL-UHFFFAOYSA-N
Formula: C10H9NO3
SMILES: O=C(O)C=CC(=O)Nc1ccccc1
Mol. weight [g/mol]: 191.19

Physical Properties

Property code	Value	Unit	Source
gf	-79.32	kJ/mol	Joback Method
hf	-219.90	kJ/mol	Joback Method
hfus	28.28	kJ/mol	Joback Method
hvap	76.69	kJ/mol	Joback Method
log10ws	-2.72		Aqueous Solubility Prediction Method
logp	1.266		Crippen Method
mcvol	142.690	ml/mol	McGowan Method
pc	4088.15	kPa	Joback Method
tb	709.13	K	Joback Method
tc	923.81	K	Joback Method
tf	437.14	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.43	J/mol×K	709.13	Joback Method
cpg	371.56	J/mol×K	744.91	Joback Method
cpg	380.00	J/mol×K	780.69	Joback Method
cpg	387.81	J/mol×K	816.47	Joback Method
cpg	395.03	J/mol×K	852.25	Joback Method
cpg	401.72	J/mol×K	888.03	Joback Method
cpg	407.92	J/mol×K	923.81	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume