2-(Benzoyloxy)-N-butylacetamide

Inchi: InChI=1S/C13H17NO3/c1-2-3-9-14-12(15)10-17-13(16)11-7-5-4-6-8-11/h4-8H,2-3,9-10H
InchiKey: FUKCEEDRHGCYHH-UHFFFAOYSA-N
Formula: C13H17NO3
SMILES: CCCCNC(=O)COC(=O)c1ccccc1
Mol. weight [g/mol]: 235.28

Physical Properties

Property code	Value	Unit	Source
gf	-102.46	kJ/mol	Joback Method
hf	-379.03	kJ/mol	Joback Method
hfus	32.95	kJ/mol	Joback Method
hvap	69.15	kJ/mol	Joback Method
log10ws	-2.76		Aqueous Solubility Prediction Method
logp	1.760		Crippen Method
mcvol	189.260	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
tb	703.85	K	Joback Method
tc	913.50	K	Joback Method
tf	342.65	K	Aqueous Solubility Prediction Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.92	J/mol×K	703.85	Joback Method
cpg	528.77	J/mol×K	738.79	Joback Method
cpg	541.70	J/mol×K	773.73	Joback Method
cpg	553.73	J/mol×K	808.68	Joback Method
cpg	564.89	J/mol×K	843.62	Joback Method
cpg	575.21	J/mol×K	878.56	Joback Method
cpg	584.72	J/mol×K	913.50	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