Benzoic acid, 4-[(1,3-dioxobutyl)amino]-

Other names: p-Carboxyacetoacetanilide
Inchi: InChI=1S/C11H11NO4/c1-7(13)6-10(14)12-9-4-2-8(3-5-9)11(15)16/h2-5H,6H2,1H3,(H,12
InchiKey: NTVPMGIWCMTNMD-UHFFFAOYSA-N
Formula: C11H11NO4
SMILES: CC(=O)CC(=O)Nc1ccc(C(=O)O)cc1
Mol. weight [g/mol]: 221.21
CAS: 34376-24-4

Physical Properties

Property code	Value	Unit	Source
gf	-289.67	kJ/mol	Joback Method
hf	-481.81	kJ/mol	Joback Method
hfus	31.88	kJ/mol	Joback Method
hvap	86.37	kJ/mol	Joback Method
log10ws	-1.85		Crippen Method
logp	1.302		Crippen Method
mcvol	162.650	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
tb	786.70	K	Joback Method
tc	998.68	K	Joback Method
tf	515.94	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.92	J/mol×K	786.70	Joback Method
cpg	452.87	J/mol×K	822.03	Joback Method
cpg	461.12	J/mol×K	857.36	Joback Method
cpg	468.70	J/mol×K	892.69	Joback Method
cpg	475.63	J/mol×K	928.02	Joback Method
cpg	481.94	J/mol×K	963.35	Joback Method
cpg	487.68	J/mol×K	998.68	Joback Method

Sources

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=C34376244&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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