P-ACETOACETAMIDOBENZOIC ACID

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

Physical Properties

Property code	Value	Unit	Source
hf	-640.71	kJ/mol	Cheméo Relay (1.0)
hfus	31.88	kJ/mol	Joback Method
hvap	111.59	kJ/mol	Cheméo Relay (1.0)
ie	8.43	eV	Cheméo Relay (1.0)
log10ws	-1.85		Cheméo Relay (1.0)
logp	1.302		Crippen Method
mcvol	162.650	ml/mol	McGowan Method
tb	613.35	K	Cheméo Relay (1.0)
tc	903.05	K	Cheméo Relay (1.0)
tf	479.89	K	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C34376244&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

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point