Deanol acetamidobenzoate

Other names: 4-(acetamido)benzoic acid, compound with 2-(dimethylamino)ethanol (1:1)
Inchi: InChI=1S/C9H9NO3/c1-6(11)10-8-4-2-7(3-5-8)9(12)13/h2-5H,1H3,(H,10,11)(H,12,13)
InchiKey: QCXJEYYXVJIFCE-UHFFFAOYSA-N
Formula: C9H9NO3
SMILES: CC(=O)Nc1ccc(C(=O)O)cc1
Mol. weight [g/mol]: 179.17
CAS: 3635-74-3

Physical Properties

Property code	Value	Unit	Source
gf	-177.59	kJ/mol	Joback Method
hf	-327.95	kJ/mol	Joback Method
hfus	25.10	kJ/mol	Joback Method
hvap	75.17	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.343		Crippen Method
mcvol	132.900	ml/mol	McGowan Method
pc	4244.08	kPa	Joback Method
rinpol	2227.00		NIST Webbook
rinpol	2227.00		NIST Webbook
tb	687.07	K	Joback Method
tc	898.02	K	Joback Method
tf	443.47	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.53	J/mol×K	687.07	Joback Method
cpg	344.57	J/mol×K	722.23	Joback Method
cpg	352.97	J/mol×K	757.39	Joback Method
cpg	360.77	J/mol×K	792.54	Joback Method
cpg	367.97	J/mol×K	827.70	Joback Method
cpg	374.62	J/mol×K	862.86	Joback Method

cpg	380.73	J/mol×K	898.02	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=C3635743&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