Benzenebutanoic acid, «alpha»,2-diamino-«gamma»-oxo-

Other names: Alanine, 3-anthraniloyl-
Kynurenin
Kynurenine
Quinurenine
3-Anthraniloylalanine
dl-Kynurenine
«alpha»-2-diamino-«gamma»-oxobenzenebutyric acid

Inchi: InChI=1S/C10H12N2O3/c11-7-4-2-1-3-6(7)9(13)5-8(12)10(14)15/h1-4,8H,5,11-12H2,(H,

InchiKey: YGPSJZOEDVAXAB-UHFFFAOYSA-N

Formula: C10H12N2O3

SMILES: Nc1ccccc1C(=O)CC(N)C(=O)O

Mol. weight [g/mol]: 208.21

CAS: 343-65-7

Physical Properties

Property code	Value	Unit	Source
gf	-128.10	kJ/mol	Joback Method
hf	-339.76	kJ/mol	Joback Method
hfus	29.46	kJ/mol	Joback Method
hvap	91.86	kJ/mol	Joback Method
log10ws	-1.25		Crippen Method
logp	0.254		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
tb	804.40	K	Joback Method
tc	1028.91	K	Joback Method
tf	553.60	K	Joback Method
vc	0.571	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	444.23	J/mol×K	804.40	Joback Method
cpg	453.07	J/mol×K	841.82	Joback Method

cpg	461.19	J/mol×K	879.24	Joback Method
cpg	468.61	J/mol×K	916.65	Joback Method
cpg	475.38	J/mol×K	954.07	Joback Method
cpg	481.54	J/mol×K	991.49	Joback Method
cpg	487.12	J/mol×K	1028.91	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=C343657&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume