3-ANTHRANILOYL-L-ALANINE

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)C[C@H](N)C(=O)O
Mol. weight [g/mol]: 208.22

Physical Properties

Property code	Value	Unit	Source
hf	-436.10	kJ/mol	Cheméo Relay (1.0)
hfus	29.46	kJ/mol	Joback Method
ie	8.11	eV	Cheméo Relay (1.0)
log10ws	-1.71		Cheméo Relay (1.0)
logp	0.254		Crippen Method
mcvol	156.970	ml/mol	McGowan Method
tb	630.07	K	Cheméo Relay (1.0)
tf	500.67	K	Cheméo Relay (1.0)

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2922830&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point