

DL-ETHYL 2-ACETAMIDO-3-PHENYLPROPIONATE

Other names:	(dl) N-acetylphenylalanine, ether ester ethyl 2-acetamido-3-phenylpropanoate
Inchi:	InChI=1S/C13H17NO3/c1-3-17-13(16)12(14-10(2)15)9-11-7-5-4-6-8-11/h4-8,12H,3,9H2,
InchiKey:	YIVZYFDBEPMPNL-UHFFFAOYSA-N
Formula:	C13H17NO3
SMILES:	CCOC(=O)C(Cc1ccccc1)NC(C)=O
Mol. weight [g/mol]:	235.28

Physical Properties

Property code	Value	Unit	Source
af	0.6137		Cheméo Relay (1.0)
hfus	29.43	kJ/mol	Joback Method
hvap	89.22	kJ/mol	Cheméo Relay (1.0)
ie	8.74	eV	Cheméo Relay (1.0)
log10ws	-1.86		Aqueous Solubility Prediction Method
logp	1.297		Crippen Method
mcvol	189.260	ml/mol	McGowan Method
pc	2487.55	kPa	Joback Method
tb	585.29	K	Cheméo Relay (1.0)
tc	794.34	K	Cheméo Relay (1.0)
tf	322.22	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.47	J/mol×K	703.41	Joback Method
cpg	529.58	J/mol×K	738.96	Joback Method
cpg	542.73	J/mol×K	774.52	Joback Method
cpg	554.94	J/mol×K	810.07	Joback Method
cpg	566.24	J/mol×K	845.63	Joback Method
cpg	576.66	J/mol×K	881.18	Joback Method
cpg	586.23	J/mol×K	916.73	Joback Method
hvapt	82.40	kJ/mol	483.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4134092&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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

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