

2-AMINO-3-PHENYLPROPIONIC ACID, ETHYL ESTER

Inchi:	InChI=1S/C11H15NO2/c1-3-14-11(13)9(2)12-10-7-5-4-6-8-10/h4-9,12H,3H2,1-2H3
InchiKey:	FMFDWCAQDWISCD-UHFFFAOYSA-N
Formula:	C11H15NO2
SMILES:	CCOC(=O)C(C)Nc1ccccc1
Mol. weight [g/mol]:	193.25

Physical Properties

Property code	Value	Unit	Source
af	0.5248		Cheméo Relay (1.0)
hf	-325.88	kJ/mol	Cheméo Relay (1.0)
hfus	22.65	kJ/mol	Joback Method
hvap	73.25	kJ/mol	Cheméo Relay (1.0)
ie	7.79	eV	Cheméo Relay (1.0)
log10ws	-2.35		Cheméo Relay (1.0)
logp	2.050		Crippen Method
mcvol	159.510	ml/mol	McGowan Method
pc	2841.41	kPa	Joback Method
tb	537.58	K	Cheméo Relay (1.0)
tc	757.88	K	Cheméo Relay (1.0)
tf	319.69	K	Cheméo Relay (1.0)
vc	0.567	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.75	J/mol×K	603.78	Joback Method
cpg	411.36	J/mol×K	639.37	Joback Method
cpg	425.07	J/mol×K	674.96	Joback Method
cpg	437.92	J/mol×K	710.54	Joback Method
cpg	449.93	J/mol×K	746.13	Joback Method
cpg	461.11	J/mol×K	781.72	Joback Method
cpg	471.50	J/mol×K	817.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1795966&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

af:	Acentric Factor
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
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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