L-«alpha»-Aminobutyric acid, N-ethoxycarbonyl, (S)-1-phenylethylamide

Inchi: InChI=1S/C15H22N2O3/c1-4-13(17-15(19)20-5-2)14(18)16-11(3)12-9-7-6-8-10-12/h6-11

InchiKey: OZEQGPIMDHVKDV-AAEUAGOBSA-N

Formula: C15H22N2O3

SMILES: CCOC(=O)NC(CC)C(=O)NC(C)c1ccccc1

Mol. weight [g/mol]: 278.35

Physical Properties

Property code	Value	Unit	Source
gf	-1.11	kJ/mol	Joback Method
hf	-377.40	kJ/mol	Joback Method
hfus	36.18	kJ/mol	Joback Method
hvap	79.26	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	2.388		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	2081.00		NIST Webbook
tb	798.90	K	Joback Method
tc	1010.75	K	Joback Method
tf	482.64	K	Joback Method
vc	0.856	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.62	J/mol×K	798.90	Joback Method
cpg	692.87	J/mol×K	834.21	Joback Method
cpg	706.04	J/mol×K	869.52	Joback Method
cpg	718.18	J/mol×K	904.83	Joback Method
cpg	729.33	J/mol×K	940.14	Joback Method
cpg	739.52	J/mol×K	975.45	Joback Method
cpg	748.79	J/mol×K	1010.75	Joback Method

Sources

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=R587543&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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