L-«beta»-Aminoisobutyric acid, N-ethoxycarbonyl, (S)-1-phenylethylamide

Inchi: InChI=1S/C15H22N2O3/c1-4-20-15(19)16-10-11(2)14(18)17-12(3)13-8-6-5-7-9-13/h5-9,1

InchiKey: ZWRSZYOWSZHTTM-PIJUOVFKSA-N

Formula: C15H22N2O3

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

Mol. weight [g/mol]: 278.35

Physical Properties

Property code	Value	Unit	Source
af	0.7120		Cheméo Relay (1.0)
hfus	36.18	kJ/mol	Joback Method
hvap	107.91	kJ/mol	Cheméo Relay (1.0)
ie	8.59	eV	Cheméo Relay (1.0)
log10ws	-2.38		Cheméo Relay (1.0)
logp	2.246		Crippen Method
mcvol	227.420	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	2160.00		NIST Webbook
tb	588.25	K	Cheméo Relay (1.0)
tc	842.75	K	Cheméo Relay (1.0)
tf	366.47	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R587558&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

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point