D-2-Phenylglycine, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi: InChI=1S/C16H23NO4/c1-5-20-16(19)17-14(13-9-7-6-8-10-13)15(18)21-12(4)11(2)3/h6-1

InchiKey: WCLRJFYIEARGAI-PUODRLBUSA-N

Formula: C16H23NO4

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

Mol. weight [g/mol]: 293.36

Physical Properties

Property code	Value	Unit	Source
gf	-189.52	kJ/mol	Joback Method
hf	-589.01	kJ/mol	Joback Method
hfus	31.34	kJ/mol	Joback Method
hvap	77.07	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.061		Crippen Method
mcvol	237.400	ml/mol	McGowan Method
pc	1900.26	kPa	Joback Method
rinpol	1932.10		NIST Webbook
tb	793.59	K	Joback Method
tc	1004.49	K	Joback Method
tf	448.48	K	Joback Method
vc	0.888	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	707.27	J/mol×K	793.59	Joback Method
cpg	722.34	J/mol×K	828.74	Joback Method
cpg	736.26	J/mol×K	863.89	Joback Method
cpg	749.06	J/mol×K	899.04	Joback Method
cpg	760.77	J/mol×K	934.19	Joback Method
cpg	771.39	J/mol×K	969.34	Joback Method
cpg	780.97	J/mol×K	1004.49	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=R501772&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