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

Inchi: InChI=1S/C17H25NO4/c1-5-21-17(20)18-15(11-14-9-7-6-8-10-14)16(19)22-13(4)12(2)3/h

InchiKey: XOBNYRVITXPDDJ-AFYYWNPRSA-N

Formula: C17H25NO4

SMILES: CCOC(=O)NC(Cc1ccccc1)C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 307.38

Physical Properties

Property code	Value	Unit	Source
gf	-181.10	kJ/mol	Joback Method
hf	-609.65	kJ/mol	Joback Method
hfus	33.93	kJ/mol	Joback Method
hvap	79.30	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	2.931		Crippen Method
mcvol	251.490	ml/mol	McGowan Method
pc	1750.67	kPa	Joback Method
rinpol	2026.90		NIST Webbook
rinpol	2026.90		NIST Webbook
tb	816.47	K	Joback Method
tc	1025.89	K	Joback Method
tf	459.75	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.08	J/mol×K	816.47	Joback Method
cpg	779.31	J/mol×K	851.37	Joback Method
cpg	793.38	J/mol×K	886.28	Joback Method
cpg	806.30	J/mol×K	921.18	Joback Method
cpg	818.10	J/mol×K	956.08	Joback Method
cpg	828.80	J/mol×K	990.98	Joback Method
cpg	838.43	J/mol×K	1025.89	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=R501925&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