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

Inchi: InChI=1S/C20H29NO7/c1-6-25-19(23)21-17(18(22)27-14(5)13(3)4)12-15-8-10-16(11-9-1

InchiKey: WBYTUPSDDYAAMZ-XPCCGILXSA-N

Formula: C20H29NO7

SMILES: CCOC(=O)NC(Cc1ccc(OC(=O)OCC)cc1)C(=O)OC(C)C(C)C

Mol. weight [g/mol]: 395.45

Physical Properties

Property code	Value	Unit	Source
gf	-504.39	kJ/mol	Joback Method
hf	-1060.06	kJ/mol	Joback Method
hfus	45.29	kJ/mol	Joback Method
hvap	98.20	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.467		Crippen Method
mcvol	307.070	ml/mol	McGowan Method
pc	1409.07	kPa	Joback Method
rinpol	2549.90		NIST Webbook
rinpol	2549.90		NIST Webbook
tb	988.80	K	Joback Method
tc	1212.28	K	Joback Method
tf	600.47	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1005.48	J/mol×K	988.80	Joback Method
cpg	1017.06	J/mol×K	1026.05	Joback Method
cpg	1026.92	J/mol×K	1063.29	Joback Method
cpg	1035.07	J/mol×K	1100.54	Joback Method
cpg	1041.50	J/mol×K	1137.79	Joback Method
cpg	1046.21	J/mol×K	1175.04	Joback Method
cpg	1049.19	J/mol×K	1212.28	Joback Method

Sources

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=R501970&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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