«alpha»-Aminopimelic acid, N(O,S)-ethoxycarbonyl, (S)-(+)-3-methyl-2-butyl ester

Inchi: InChI=1S/C20H37NO6/c1-8-25-20(24)21-17(19(23)27-16(7)14(4)5)11-9-10-12-18(22)26-

InchiKey: YCHVHIFLTBDCOA-YNPPLXCJSA-N

Formula: C20H37NO6

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

Mol. weight [g/mol]: 387.51

Physical Properties

Property code	Value	Unit	Source
gf	-507.05	kJ/mol	Joback Method
hf	-1163.46	kJ/mol	Joback Method
hfus	43.40	kJ/mol	Joback Method
hvap	92.08	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.837		Crippen Method
mcvol	324.960	ml/mol	McGowan Method
pc	1151.44	kPa	Joback Method
rinpol	2349.10		NIST Webbook
rinpol	2357.50		NIST Webbook
tb	933.84	K	Joback Method
tc	1143.53	K	Joback Method
tf	509.30	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1085.03	J/mol×K	933.84	Joback Method
cpg	1100.63	J/mol×K	968.79	Joback Method
cpg	1114.72	J/mol×K	1003.74	Joback Method
cpg	1127.33	J/mol×K	1038.69	Joback Method
cpg	1138.45	J/mol×K	1073.64	Joback Method
cpg	1148.12	J/mol×K	1108.58	Joback Method
cpg	1156.32	J/mol×K	1143.53	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=R501707&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