L-2,3-Diaminopropionic acid, N-ethoxycarbonyl, (S)-1-phenylethylamide

Inchi: InChI=1S/C17H25N3O5/c1-4-24-16(22)18-11-14(20-17(23)25-5-2)15(21)19-12(3)13-9-7-

InchiKey: VPHQYHMUSQAPPH-TZMCWYRMSA-N

Formula: C17H25N3O5

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

Mol. weight [g/mol]: 351.40

Physical Properties

Property code	Value	Unit	Source
gf	-128.80	kJ/mol	Joback Method
hf	-610.01	kJ/mol	Joback Method
hfus	49.25	kJ/mol	Joback Method
hvap	99.30	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	1.725		Crippen Method
mcvol	273.020	ml/mol	McGowan Method
pc	1875.65	kPa	Joback Method
rinpol	2539.00		NIST Webbook
rinpol	2539.00		NIST Webbook
tb	971.12	K	Joback Method
tc	1194.06	K	Joback Method
tf	630.00	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	884.92	J/mol×K	971.12	Joback Method
cpg	896.01	J/mol×K	1008.28	Joback Method
cpg	905.79	J/mol×K	1045.43	Joback Method
cpg	914.30	J/mol×K	1082.59	Joback Method
cpg	921.58	J/mol×K	1119.75	Joback Method
cpg	927.65	J/mol×K	1156.91	Joback Method
cpg	932.55	J/mol×K	1194.06	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=R587563&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