L-Aspartic acid, N-methyl, N-ethoxycarbonyl, (S)-1-phenylethylamide

Inchi: InChI=1S/C24H31N3O4/c1-5-31-24(30)27(4)21(23(29)26-18(3)20-14-10-7-11-15-20)16-2

InchiKey: KWSQQULDQQMNPS-WAOWUJCRSA-N

Formula: C24H31N3O4

SMILES: CCOC(=O)N(C)C(CC(=O)NC(C)c1ccccc1)C(=O)NC(C)c1ccccc1

Mol. weight [g/mol]: 425.52

Physical Properties

Property code	Value	Unit	Source
gf	166.50	kJ/mol	Joback Method
hf	-376.96	kJ/mol	Joback Method
hfus	54.63	kJ/mol	Joback Method
hvap	109.97	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	3.588		Crippen Method
mcvol	342.020	ml/mol	McGowan Method
pc	1434.80	kPa	Joback Method
rinpol	3170.00		NIST Webbook
tb	1097.37	K	Joback Method
tc	1344.27	K	Joback Method
tf	677.89	K	Joback Method
vc	1.270	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1152.12	J/mol×K	1097.37	Joback Method
cpg	1163.51	J/mol×K	1138.52	Joback Method
cpg	1173.65	J/mol×K	1179.67	Joback Method
cpg	1182.66	J/mol×K	1220.82	Joback Method
cpg	1190.66	J/mol×K	1261.97	Joback Method
cpg	1197.79	J/mol×K	1303.12	Joback Method
cpg	1204.16	J/mol×K	1344.27	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R587583&Units=SI

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