L-Ile, N-ethoxycarbonyl, (S)-1-phenylethylamide

Inchi: InChI=1S/C17H26N2O3/c1-5-12(3)15(19-17(21)22-6-2)16(20)18-13(4)14-10-8-7-9-11-14

InchiKey: GDBUWMVLQLZXQU-YDHLFZDLSA-N

Formula: C17H26N2O3

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

Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	13.29	kJ/mol	Joback Method
hf	-423.96	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	83.32	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.025		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	2190.00		NIST Webbook
tb	844.22	K	Joback Method
tc	1056.09	K	Joback Method
tf	490.18	K	Joback Method
vc	0.962	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.80	J/mol×K	844.22	Joback Method
cpg	807.62	J/mol×K	879.53	Joback Method
cpg	821.28	J/mol×K	914.84	Joback Method
cpg	833.85	J/mol×K	950.16	Joback Method
cpg	845.35	J/mol×K	985.47	Joback Method
cpg	855.83	J/mol×K	1020.78	Joback Method
cpg	865.34	J/mol×K	1056.09	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=R587598&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