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

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

InchiKey: CRTCXZPKJPQVGP-UKRRQHHQSA-N

Formula: C17H26N2O3

SMILES: CCCCC(NC(=O)OCC)C(=O)NC(C)c1ccccc1

Mol. weight [g/mol]: 306.40

Physical Properties

Property code	Value	Unit	Source
gf	15.73	kJ/mol	Joback Method
hf	-418.68	kJ/mol	Joback Method
hfus	41.36	kJ/mol	Joback Method
hvap	83.71	kJ/mol	Joback Method
log10ws	-4.61		Crippen Method
logp	3.169		Crippen Method
mcvol	255.600	ml/mol	McGowan Method
pc	1783.35	kPa	Joback Method
rinpol	2246.00		NIST Webbook
rinpol	2246.00		NIST Webbook
tb	844.66	K	Joback Method
tc	1054.17	K	Joback Method
tf	505.18	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.26	J/mol×K	844.66	Joback Method
cpg	806.93	J/mol×K	879.58	Joback Method
cpg	820.48	J/mol×K	914.50	Joback Method
cpg	832.97	J/mol×K	949.41	Joback Method
cpg	844.43	J/mol×K	984.33	Joback Method
cpg	854.90	J/mol×K	1019.25	Joback Method
cpg	864.43	J/mol×K	1054.17	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=R587612&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