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

Inchi: InChI=1S/C16H24N2O3/c1-5-21-16(20)18-14(11(2)3)15(19)17-12(4)13-9-7-6-8-10-13/h6

InchiKey: GPURSIJORGNZPY-JSGCOSHPSA-N

Formula: C16H24N2O3

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

Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	4.87	kJ/mol	Joback Method
hf	-403.32	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	81.10	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	2.634		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	2111.00		NIST Webbook
rinpol	2111.00		NIST Webbook
tb	821.34	K	Joback Method
tc	1034.39	K	Joback Method
tf	478.91	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.56	J/mol×K	821.34	Joback Method
cpg	750.20	J/mol×K	856.85	Joback Method
cpg	763.71	J/mol×K	892.36	Joback Method
cpg	776.13	J/mol×K	927.86	Joback Method
cpg	787.51	J/mol×K	963.37	Joback Method
cpg	797.88	J/mol×K	998.88	Joback Method
cpg	807.29	J/mol×K	1034.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R587652&Units=SI
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

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