D-Norval, N-ethoxycarbonyl, (S)-1-phenylethylamide

Inchi: InChI=1S/C16H24N2O3/c1-4-9-14(18-16(20)21-5-2)15(19)17-12(3)13-10-7-6-8-11-13/h6
InchiKey: ZNDAJFRHIWRDFF-GXTWGEPZSA-N
Formula: C16H24N2O3
SMILES: CCCC(NC(=O)OCC)C(=O)NC(C)c1ccccc1
Mol. weight [g/mol]: 292.37

Physical Properties

Property code	Value	Unit	Source
gf	7.31	kJ/mol	Joback Method
hf	-398.04	kJ/mol	Joback Method
hfus	38.77	kJ/mol	Joback Method
hvap	81.48	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	2.779		Crippen Method
mcvol	241.510	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	2132.00		NIST Webbook
rinpol	2132.00		NIST Webbook
tb	821.78	K	Joback Method
tc	1032.15	K	Joback Method
tf	493.91	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	735.00	J/mol×K	821.78	Joback Method
cpg	749.47	J/mol×K	856.84	Joback Method
cpg	762.84	J/mol×K	891.90	Joback Method
cpg	775.17	J/mol×K	926.96	Joback Method
cpg	786.49	J/mol×K	962.02	Joback Method
cpg	796.84	J/mol×K	997.09	Joback Method
cpg	806.25	J/mol×K	1032.15	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=R587503&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