L-Norvaline, N-butoxycarbonyl-, tetradecyl ester

Inchi: InChI=1S/C24H47NO4/c1-4-7-9-10-11-12-13-14-15-16-17-18-21-28-23(26)22(19-6-3)25-

InchiKey: ZMMTYOUQQZBHTJ-UHFFFAOYSA-N

Formula: C24H47NO4

SMILES: CCCCCCCCCCCCCCOC(=O)C(CCC)NC(=O)OCCCC

Mol. weight [g/mol]: 413.64

Physical Properties

Property code	Value	Unit	Source
af	1.1953		Cheméo Relay (1.0)
hf	-1148.65	kJ/mol	Cheméo Relay (1.0)
hfus	65.07	kJ/mol	Joback Method
hvap	121.53	kJ/mol	Cheméo Relay (1.0)
ie	9.17	eV	Cheméo Relay (1.0)
log10ws	-6.68		Cheméo Relay (1.0)
logp	6.926		Crippen Method
mcvol	373.880	ml/mol	McGowan Method
pc	860.49	kPa	Joback Method
tb	635.97	K	Cheméo Relay (1.0)
tc	839.20	K	Cheméo Relay (1.0)
tf	313.42	K	Cheméo Relay (1.0)
vc	1.419	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1283.65	J/mol×K	950.83	Joback Method
cpg	1303.36	J/mol×K	987.11	Joback Method
cpg	1321.47	J/mol×K	1023.38	Joback Method
cpg	1338.01	J/mol×K	1059.66	Joback Method
cpg	1353.04	J/mol×K	1095.94	Joback Method
cpg	1366.59	J/mol×K	1132.21	Joback Method
cpg	1378.72	J/mol×K	1168.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320780&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume