D-Alanine, N-butoxycarbonyl-, hexadecyl ester

Inchi: InChI=1S/C24H47NO4/c1-4-6-8-9-10-11-12-13-14-15-16-17-18-19-21-28-23(26)22(3)25-
InchiKey: HBZYMZNZFCEUHE-UHFFFAOYSA-N
Formula: C24H47NO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)OCCCC
Mol. weight [g/mol]: 413.63

Physical Properties

Property code	Value	Unit	Source
gf	-229.69	kJ/mol	Joback Method
hf	-980.10	kJ/mol	Joback Method
hfus	65.07	kJ/mol	Joback Method
hvap	93.38	kJ/mol	Joback Method
log10ws	-7.87		Crippen Method
logp	6.926		Crippen Method
mcvol	373.880	ml/mol	McGowan Method
pc	860.49	kPa	Joback Method
rinpol	2838.00		NIST Webbook
tb	950.83	K	Joback Method
tc	1168.49	K	Joback Method
tf	542.22	K	Joback Method
vc	1.456	m3/kmol	Joback Method

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

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=U347730&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