DL-Alanine, N-methyl-N-decyloxycarbonyl-, butyl ester

Inchi: InChI=1S/C19H37NO4/c1-5-7-9-10-11-12-13-14-16-24-19(22)20(4)17(3)18(21)23-15-8-6

InchiKey: ZBEFHQYKSCPJQQ-UHFFFAOYSA-N

Formula: C19H37NO4

SMILES: CCCCCCCCCCOC(=O)N(C)C(C)C(=O)OCCCC

Mol. weight [g/mol]: 343.50

Physical Properties

Property code	Value	Unit	Source
gf	-250.40	kJ/mol	Joback Method
hf	-862.84	kJ/mol	Joback Method
hfus	50.04	kJ/mol	Joback Method
hvap	77.86	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.927		Crippen Method
mcvol	303.430	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	2213.00		NIST Webbook
rinpol	2213.00		NIST Webbook
tb	798.70	K	Joback Method
tc	981.66	K	Joback Method
tf	465.68	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.38	J/mol×K	798.70	Joback Method
cpg	970.45	J/mol×K	829.19	Joback Method
cpg	987.50	J/mol×K	859.69	Joback Method
cpg	1003.53	J/mol×K	890.18	Joback Method
cpg	1018.56	J/mol×K	920.67	Joback Method
cpg	1032.62	J/mol×K	951.16	Joback Method
cpg	1045.73	J/mol×K	981.66	Joback Method

Sources

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=U392674&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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