L-Valine, N-(2-methoxybenzoyl)-, hexadecyl ester

Inchi: InChI=1S/C29H49NO4/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-20-23-34-29(32)27(24(2)3
InchiKey: QZXDGETZVVCEMQ-UHFFFAOYSA-N
Formula: C29H49NO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1ccccc1OC)C(C)C
Mol. weight [g/mol]: 475.70

Physical Properties

Property code	Value	Unit	Source
gf	-87.25	kJ/mol	Joback Method
hf	-863.52	kJ/mol	Joback Method
hfus	68.14	kJ/mol	Joback Method
hvap	107.06	kJ/mol	Joback Method
log10ws	-9.04		Crippen Method
logp	7.474		Crippen Method
mcvol	420.570	ml/mol	McGowan Method
pc	786.83	kPa	Joback Method
rinpol	3564.00		NIST Webbook
rinpol	3564.00		NIST Webbook
tb	1096.45	K	Joback Method
tc	1356.02	K	Joback Method
tf	622.51	K	Joback Method
vc	1.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1493.76	J/mol×K	1096.45	Joback Method
cpg	1511.07	J/mol×K	1139.71	Joback Method
cpg	1526.23	J/mol×K	1182.97	Joback Method
cpg	1539.35	J/mol×K	1226.23	Joback Method
cpg	1550.53	J/mol×K	1269.50	Joback Method
cpg	1559.88	J/mol×K	1312.76	Joback Method
cpg	1567.50	J/mol×K	1356.02	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=U346600&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