L-Valine, N-(4-methylbenzoyl)-, tetradecyl ester

Inchi: InChI=1S/C27H45NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-21-31-27(30)25(22(2)3)28-26

InchiKey: OEOHXTKWCOKHOM-UHFFFAOYSA-N

Formula: C27H45NO3

SMILES: CCCCCCCCCCCCCCOC(=O)C(NC(=O)c1ccc(C)cc1)C(C)C

Mol. weight [g/mol]: 431.65

Physical Properties

Property code	Value	Unit	Source
gf	0.91	kJ/mol	Joback Method
hf	-690.02	kJ/mol	Joback Method
hfus	61.78	kJ/mol	Joback Method
hvap	100.20	kJ/mol	Joback Method
log10ws	-8.56		Crippen Method
logp	6.994		Crippen Method
mcvol	386.520	ml/mol	McGowan Method
pc	887.88	kPa	Joback Method
rinpol	3235.00		NIST Webbook
rinpol	3235.00		NIST Webbook
tb	1028.27	K	Joback Method
tc	1260.90	K	Joback Method
tf	577.74	K	Joback Method
vc	1.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1339.18	J/mol×K	1028.27	Joback Method
cpg	1356.89	J/mol×K	1067.04	Joback Method
cpg	1373.03	J/mol×K	1105.81	Joback Method
cpg	1387.67	J/mol×K	1144.59	Joback Method
cpg	1400.92	J/mol×K	1183.36	Joback Method
cpg	1412.85	J/mol×K	1222.13	Joback Method
cpg	1423.54	J/mol×K	1260.90	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=U346646&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