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

Inchi: InChI=1S/C30H51NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-24-34-30(33)28(25(

InchiKey: WSHTZMGMWOSCRS-UHFFFAOYSA-N

Formula: C30H51NO3

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

Mol. weight [g/mol]: 473.73

Physical Properties

Property code	Value	Unit	Source
gf	26.17	kJ/mol	Joback Method
hf	-751.94	kJ/mol	Joback Method
hfus	69.55	kJ/mol	Joback Method
hvap	106.87	kJ/mol	Joback Method
log10ws	-9.82		Crippen Method
logp	8.164		Crippen Method
mcvol	428.790	ml/mol	McGowan Method
pc	753.08	kPa	Joback Method
rinpol	3559.00		NIST Webbook
rinpol	3559.00		NIST Webbook
tb	1096.91	K	Joback Method
tc	1357.24	K	Joback Method
tf	611.55	K	Joback Method
vc	1.661	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1530.10	J/mol×K	1096.91	Joback Method
cpg	1549.11	J/mol×K	1140.30	Joback Method
cpg	1566.19	J/mol×K	1183.69	Joback Method
cpg	1581.49	J/mol×K	1227.07	Joback Method
cpg	1595.15	J/mol×K	1270.46	Joback Method
cpg	1607.29	J/mol×K	1313.85	Joback Method
cpg	1618.07	J/mol×K	1357.24	Joback Method

Sources

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=U346649&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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