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

Inchi: InChI=1S/C28H47NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-22-32-28(31)26(23(2)3)29

InchiKey: KLUPCNQWDQTWPK-UHFFFAOYSA-N

Formula: C28H47NO3

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

Mol. weight [g/mol]: 445.68

Physical Properties

Property code	Value	Unit	Source
gf	9.33	kJ/mol	Joback Method
hf	-710.66	kJ/mol	Joback Method
hfus	64.37	kJ/mol	Joback Method
hvap	102.42	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	7.384		Crippen Method
mcvol	400.610	ml/mol	McGowan Method
pc	839.19	kPa	Joback Method
rinpol	3341.00		NIST Webbook
rinpol	3341.00		NIST Webbook
tb	1051.15	K	Joback Method
tc	1291.69	K	Joback Method
tf	589.01	K	Joback Method
vc	1.548	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1402.49	J/mol×K	1051.15	Joback Method
cpg	1420.58	J/mol×K	1091.24	Joback Method
cpg	1437.00	J/mol×K	1131.33	Joback Method
cpg	1451.84	J/mol×K	1171.42	Joback Method
cpg	1465.20	J/mol×K	1211.51	Joback Method
cpg	1477.19	J/mol×K	1251.60	Joback Method
cpg	1487.90	J/mol×K	1291.69	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=U346647&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

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