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

Inchi: InChI=1S/C24H39NO3/c1-5-6-7-8-9-10-11-12-13-18-28-24(27)22(19(2)3)25-23(26)21-16
InchiKey: XTRAXVUWIFCFRE-UHFFFAOYSA-N
Formula: C24H39NO3
SMILES: CCCCCCCCCCCOC(=O)C(NC(=O)c1ccc(C)cc1)C(C)C
Mol. weight [g/mol]: 389.57

Physical Properties

Property code	Value	Unit	Source
gf	-24.35	kJ/mol	Joback Method
hf	-628.10	kJ/mol	Joback Method
hfus	54.01	kJ/mol	Joback Method
hvap	93.52	kJ/mol	Joback Method
log10ws	-7.30		Crippen Method
logp	5.823		Crippen Method
mcvol	344.250	ml/mol	McGowan Method
pc	1062.40	kPa	Joback Method
rinpol	2905.00		NIST Webbook
rinpol	2905.00		NIST Webbook
tb	959.63	K	Joback Method
tc	1175.47	K	Joback Method
tf	543.93	K	Joback Method
vc	1.325	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1151.67	J/mol×K	959.63	Joback Method
cpg	1168.49	J/mol×K	995.60	Joback Method
cpg	1183.96	J/mol×K	1031.58	Joback Method
cpg	1198.15	J/mol×K	1067.55	Joback Method
cpg	1211.10	J/mol×K	1103.52	Joback Method
cpg	1222.89	J/mol×K	1139.49	Joback Method
cpg	1233.56	J/mol×K	1175.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346644&Units=SI
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

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