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

Inchi: InChI=1S/C25H41NO3/c1-5-6-7-8-9-10-11-12-13-14-19-29-25(28)23(20(2)3)26-24(27)22
InchiKey: JOMFLMSRHRLOHZ-UHFFFAOYSA-N
Formula: C25H41NO3
SMILES: CCCCCCCCCCCCOC(=O)C(NC(=O)c1ccc(C)cc1)C(C)C
Mol. weight [g/mol]: 403.60

Physical Properties

Property code	Value	Unit	Source
gf	-15.93	kJ/mol	Joback Method
hf	-648.74	kJ/mol	Joback Method
hfus	56.60	kJ/mol	Joback Method
hvap	95.74	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	6.214		Crippen Method
mcvol	358.340	ml/mol	McGowan Method
pc	998.91	kPa	Joback Method
rinpol	3013.00		NIST Webbook
rinpol	3013.00		NIST Webbook
tb	982.51	K	Joback Method
tc	1202.87	K	Joback Method
tf	555.20	K	Joback Method
vc	1.381	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.73	J/mol×K	982.51	Joback Method
cpg	1230.81	J/mol×K	1019.24	Joback Method
cpg	1246.47	J/mol×K	1055.96	Joback Method
cpg	1260.80	J/mol×K	1092.69	Joback Method
cpg	1273.84	J/mol×K	1129.42	Joback Method
cpg	1285.67	J/mol×K	1166.15	Joback Method
cpg	1296.35	J/mol×K	1202.87	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=U346645&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