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

Inchi: InChI=1S/C26H43NO3/c1-5-7-8-9-10-11-12-13-14-15-20-30-26(29)24(21(3)4)27-25(28)2
InchiKey: ZHXWXQKXVWAVCM-UHFFFAOYSA-N
Formula: C26H43NO3
SMILES: CCCCCCCCCCCCOC(=O)C(NC(=O)c1ccc(CC)cc1)C(C)C
Mol. weight [g/mol]: 417.62

Physical Properties

Property code	Value	Unit	Source
gf	-7.51	kJ/mol	Joback Method
hf	-669.38	kJ/mol	Joback Method
hfus	59.19	kJ/mol	Joback Method
hvap	97.97	kJ/mol	Joback Method
log10ws	-8.05		Crippen Method
logp	6.468		Crippen Method
mcvol	372.430	ml/mol	McGowan Method
pc	940.95	kPa	Joback Method
rinpol	3119.00		NIST Webbook
rinpol	3119.00		NIST Webbook
tb	1005.39	K	Joback Method
tc	1231.33	K	Joback Method
tf	566.47	K	Joback Method
vc	1.437	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1276.25	J/mol×K	1005.39	Joback Method
cpg	1293.62	J/mol×K	1043.05	Joback Method
cpg	1309.51	J/mol×K	1080.70	Joback Method
cpg	1323.98	J/mol×K	1118.36	Joback Method
cpg	1337.12	J/mol×K	1156.01	Joback Method
cpg	1349.00	J/mol×K	1193.67	Joback Method
cpg	1359.69	J/mol×K	1231.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U346635&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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