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

Inchi: InChI=1S/C29H49NO3/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-23-33-29(32)27(24(3)4)3
InchiKey: KYKYQTLMVNYXJL-UHFFFAOYSA-N
Formula: C29H49NO3
SMILES: CCCCCCCCCCCCCCCOC(=O)C(NC(=O)c1ccc(CC)cc1)C(C)C
Mol. weight [g/mol]: 459.70

Physical Properties

Property code	Value	Unit	Source
gf	17.75	kJ/mol	Joback Method
hf	-731.30	kJ/mol	Joback Method
hfus	66.96	kJ/mol	Joback Method
hvap	104.65	kJ/mol	Joback Method
log10ws	-9.30		Crippen Method
logp	7.638		Crippen Method
mcvol	414.700	ml/mol	McGowan Method
pc	794.39	kPa	Joback Method
rinpol	3431.00		NIST Webbook
rinpol	3431.00		NIST Webbook
tb	1074.03	K	Joback Method
tc	1323.76	K	Joback Method
tf	600.28	K	Joback Method
vc	1.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1466.14	J/mol×K	1074.03	Joback Method
cpg	1484.67	J/mol×K	1115.65	Joback Method
cpg	1501.40	J/mol×K	1157.27	Joback Method
cpg	1516.45	J/mol×K	1198.90	Joback Method
cpg	1529.95	J/mol×K	1240.52	Joback Method
cpg	1542.01	J/mol×K	1282.14	Joback Method
cpg	1552.75	J/mol×K	1323.76	Joback Method

Sources

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=U346637&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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