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

Inchi: InChI=1S/C23H37NO3/c1-5-7-8-9-10-11-12-17-27-23(26)21(18(3)4)24-22(25)20-15-13-1
InchiKey: XGZQZLLKSHKGLR-UHFFFAOYSA-N
Formula: C23H37NO3
SMILES: CCCCCCCCCOC(=O)C(NC(=O)c1ccc(CC)cc1)C(C)C
Mol. weight [g/mol]: 375.54

Physical Properties

Property code	Value	Unit	Source
gf	-32.77	kJ/mol	Joback Method
hf	-607.46	kJ/mol	Joback Method
hfus	51.42	kJ/mol	Joback Method
hvap	91.29	kJ/mol	Joback Method
log10ws	-6.79		Crippen Method
logp	5.297		Crippen Method
mcvol	330.160	ml/mol	McGowan Method
pc	1132.15	kPa	Joback Method
rinpol	2802.00		NIST Webbook
rinpol	2802.00		NIST Webbook
tb	936.75	K	Joback Method
tc	1149.04	K	Joback Method
tf	532.66	K	Joback Method
vc	1.268	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1090.11	J/mol×K	936.75	Joback Method
cpg	1106.70	J/mol×K	972.13	Joback Method
cpg	1122.00	J/mol×K	1007.51	Joback Method
cpg	1136.06	J/mol×K	1042.89	Joback Method
cpg	1148.94	J/mol×K	1078.28	Joback Method
cpg	1160.68	J/mol×K	1113.66	Joback Method
cpg	1171.35	J/mol×K	1149.04	Joback Method

Sources

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=U346632&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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