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

Inchi: InChI=1S/C21H33NO3/c1-5-7-8-9-10-15-25-21(24)19(16(3)4)22-20(23)18-13-11-17(6-2)
InchiKey: YMKJXSPJULOMNO-UHFFFAOYSA-N
Formula: C21H33NO3
SMILES: CCCCCCCOC(=O)C(NC(=O)c1ccc(CC)cc1)C(C)C
Mol. weight [g/mol]: 347.49

Physical Properties

Property code	Value	Unit	Source
gf	-49.61	kJ/mol	Joback Method
hf	-566.18	kJ/mol	Joback Method
hfus	46.24	kJ/mol	Joback Method
hvap	86.84	kJ/mol	Joback Method
log10ws	-5.96		Crippen Method
logp	4.517		Crippen Method
mcvol	301.980	ml/mol	McGowan Method
pc	1293.93	kPa	Joback Method
rinpol	2611.00		NIST Webbook
rinpol	2611.00		NIST Webbook
tb	890.99	K	Joback Method
tc	1098.86	K	Joback Method
tf	510.12	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	968.72	J/mol×K	890.99	Joback Method
cpg	984.92	J/mol×K	925.64	Joback Method
cpg	999.91	J/mol×K	960.28	Joback Method
cpg	1013.75	J/mol×K	994.93	Joback Method
cpg	1026.46	J/mol×K	1029.57	Joback Method
cpg	1038.11	J/mol×K	1064.22	Joback Method
cpg	1048.74	J/mol×K	1098.86	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=U346631&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