«beta»-Alanine, N-(4-fluorobenzoyl)-, octyl ester

Inchi: InChI=1S/C18H26FNO3/c1-2-3-4-5-6-7-14-23-17(21)12-13-20-18(22)15-8-10-16(19)11-9

InchiKey: NZYLPGXJJSQAPE-UHFFFAOYSA-N

Formula: C18H26FNO3

SMILES: CCCCCCCCOC(=O)CCNC(=O)c1ccc(F)cc1

Mol. weight [g/mol]: 323.40

Physical Properties

Property code	Value	Unit	Source
gf	-264.80	kJ/mol	Joback Method
hf	-689.81	kJ/mol	Joback Method
hfus	48.59	kJ/mol	Joback Method
hvap	80.12	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	3.849		Crippen Method
mcvol	261.480	ml/mol	McGowan Method
pc	1534.26	kPa	Joback Method
rinpol	2464.00		NIST Webbook
rinpol	2464.00		NIST Webbook
tb	822.50	K	Joback Method
tc	1020.35	K	Joback Method
tf	506.90	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.17	J/mol×K	822.50	Joback Method
cpg	813.05	J/mol×K	855.48	Joback Method
cpg	826.93	J/mol×K	888.45	Joback Method
cpg	839.84	J/mol×K	921.43	Joback Method
cpg	851.82	J/mol×K	954.40	Joback Method
cpg	862.89	J/mol×K	987.38	Joback Method
cpg	873.09	J/mol×K	1020.35	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=U321760&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