«beta»-Alanine, N-(2,6-difluorobenzoyl)-, octyl ester

Inchi: InChI=1S/C18H25F2NO3/c1-2-3-4-5-6-7-13-24-16(22)11-12-21-18(23)17-14(19)9-8-10-1

InchiKey: JQLJFGCQCPMRSE-UHFFFAOYSA-N

Formula: C18H25F2NO3

SMILES: CCCCCCCCOC(=O)CCNC(=O)c1c(F)cccc1F

Mol. weight [g/mol]: 341.39

Physical Properties

Property code	Value	Unit	Source
gf	-469.24	kJ/mol	Joback Method
hf	-897.39	kJ/mol	Joback Method
hfus	51.28	kJ/mol	Joback Method
hvap	79.97	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	3.988		Crippen Method
mcvol	263.250	ml/mol	McGowan Method
pc	1464.61	kPa	Joback Method
rinpol	2478.00		NIST Webbook
rinpol	2478.00		NIST Webbook
tb	826.75	K	Joback Method
tc	1021.49	K	Joback Method
tf	520.01	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.80	J/mol×K	826.75	Joback Method
cpg	819.22	J/mol×K	859.21	Joback Method
cpg	832.67	J/mol×K	891.66	Joback Method
cpg	845.18	J/mol×K	924.12	Joback Method
cpg	856.78	J/mol×K	956.58	Joback Method
cpg	867.50	J/mol×K	989.03	Joback Method
cpg	877.36	J/mol×K	1021.49	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=U321846&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