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

Inchi: InChI=1S/C19H27F2NO3/c1-2-3-4-5-6-7-8-14-25-17(23)12-13-22-19(24)18-15(20)10-9-1

InchiKey: XMCVARWLUFTEIC-UHFFFAOYSA-N

Formula: C19H27F2NO3

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

Mol. weight [g/mol]: 355.42

Physical Properties

Property code	Value	Unit	Source
gf	-460.82	kJ/mol	Joback Method
hf	-918.03	kJ/mol	Joback Method
hfus	53.87	kJ/mol	Joback Method
hvap	82.19	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	4.378		Crippen Method
mcvol	277.340	ml/mol	McGowan Method
pc	1362.64	kPa	Joback Method
rinpol	2580.00		NIST Webbook
rinpol	2580.00		NIST Webbook
tb	849.63	K	Joback Method
tc	1046.00	K	Joback Method
tf	531.28	K	Joback Method
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.90	J/mol×K	849.63	Joback Method
cpg	877.64	J/mol×K	882.36	Joback Method
cpg	891.38	J/mol×K	915.09	Joback Method
cpg	904.13	J/mol×K	947.82	Joback Method
cpg	915.94	J/mol×K	980.55	Joback Method
cpg	926.83	J/mol×K	1013.27	Joback Method
cpg	936.82	J/mol×K	1046.00	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=U321847&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