«beta»-Alanine, N-(3-fluorobenzoyl)-, decyl ester

Inchi: InChI=1S/C20H30FNO3/c1-2-3-4-5-6-7-8-9-15-25-19(23)13-14-22-20(24)17-11-10-12-18

InchiKey: PAYWLXBEXQGXRX-UHFFFAOYSA-N

Formula: C20H30FNO3

SMILES: CCCCCCCCCCOC(=O)CCNC(=O)c1cccc(F)c1

Mol. weight [g/mol]: 351.46

Physical Properties

Property code	Value	Unit	Source
gf	-247.96	kJ/mol	Joback Method
hf	-731.09	kJ/mol	Joback Method
hfus	53.77	kJ/mol	Joback Method
hvap	84.57	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	4.630		Crippen Method
mcvol	289.660	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
rinpol	2651.00		NIST Webbook
rinpol	2651.00		NIST Webbook
tb	868.26	K	Joback Method
tc	1068.64	K	Joback Method
tf	529.44	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.25	J/mol×K	868.26	Joback Method
cpg	930.70	J/mol×K	901.66	Joback Method
cpg	945.08	J/mol×K	935.05	Joback Method
cpg	958.41	J/mol×K	968.45	Joback Method
cpg	970.74	J/mol×K	1001.85	Joback Method
cpg	982.10	J/mol×K	1035.24	Joback Method
cpg	992.54	J/mol×K	1068.64	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=U321940&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