«beta»-Alanine, N-(2,3,4-trifluorobenzoyl)-, decyl ester

Inchi: InChI=1S/C20H28F3NO3/c1-2-3-4-5-6-7-8-9-14-27-17(25)12-13-24-20(26)15-10-11-16(2

InchiKey: KVYSKKXHWZASQO-UHFFFAOYSA-N

Formula: C20H28F3NO3

SMILES: CCCCCCCCCCOC(=O)CCNC(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 387.44

Physical Properties

Property code	Value	Unit	Source
gf	-656.84	kJ/mol	Joback Method
hf	-1146.25	kJ/mol	Joback Method
hfus	59.16	kJ/mol	Joback Method
hvap	84.26	kJ/mol	Joback Method
log10ws	-6.70		Crippen Method
logp	4.908		Crippen Method
mcvol	293.200	ml/mol	McGowan Method
pc	1218.29	kPa	Joback Method
rinpol	2561.00		NIST Webbook
rinpol	2561.00		NIST Webbook
tb	876.76	K	Joback Method
tc	1074.69	K	Joback Method
tf	555.66	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	928.27	J/mol×K	876.76	Joback Method
cpg	943.03	J/mol×K	909.75	Joback Method
cpg	956.75	J/mol×K	942.74	Joback Method
cpg	969.44	J/mol×K	975.72	Joback Method
cpg	981.13	J/mol×K	1008.71	Joback Method
cpg	991.86	J/mol×K	1041.70	Joback Method
cpg	1001.65	J/mol×K	1074.69	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=U321697&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