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

Inchi: InChI=1S/C18H24F3NO3/c1-2-3-4-5-6-7-12-25-15(23)10-11-22-18(24)13-8-9-14(19)17(2

InchiKey: NGRMXYWTAFLVNS-UHFFFAOYSA-N

Formula: C18H24F3NO3

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

Mol. weight [g/mol]: 359.38

Physical Properties

Property code	Value	Unit	Source
gf	-673.68	kJ/mol	Joback Method
hf	-1104.97	kJ/mol	Joback Method
hfus	53.97	kJ/mol	Joback Method
hvap	79.81	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	4.128		Crippen Method
mcvol	265.020	ml/mol	McGowan Method
pc	1399.59	kPa	Joback Method
rinpol	2353.00		NIST Webbook
rinpol	2353.00		NIST Webbook
tb	831.00	K	Joback Method
tc	1023.36	K	Joback Method
tf	533.12	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.39	J/mol×K	831.00	Joback Method
cpg	825.40	J/mol×K	863.06	Joback Method
cpg	838.47	J/mol×K	895.12	Joback Method
cpg	850.62	J/mol×K	927.18	Joback Method
cpg	861.89	J/mol×K	959.24	Joback Method
cpg	872.29	J/mol×K	991.30	Joback Method
cpg	881.83	J/mol×K	1023.36	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=U321695&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