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

Inchi: InChI=1S/C17H22F3NO3/c1-2-3-4-5-6-11-24-14(22)9-10-21-17(23)12-7-8-13(18)16(20)1

InchiKey: CHDVTBPGAIZIEZ-UHFFFAOYSA-N

Formula: C17H22F3NO3

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

Mol. weight [g/mol]: 345.36

Physical Properties

Property code	Value	Unit	Source
gf	-682.10	kJ/mol	Joback Method
hf	-1084.33	kJ/mol	Joback Method
hfus	51.38	kJ/mol	Joback Method
hvap	77.59	kJ/mol	Joback Method
log10ws	-5.44		Crippen Method
logp	3.737		Crippen Method
mcvol	250.930	ml/mol	McGowan Method
pc	1505.81	kPa	Joback Method
rinpol	2254.00		NIST Webbook
tb	808.12	K	Joback Method
tc	998.84	K	Joback Method
tf	521.85	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	754.20	J/mol×K	808.12	Joback Method
cpg	767.82	J/mol×K	839.91	Joback Method
cpg	780.56	J/mol×K	871.69	Joback Method
cpg	792.43	J/mol×K	903.48	Joback Method
cpg	803.46	J/mol×K	935.26	Joback Method
cpg	813.65	J/mol×K	967.05	Joback Method
cpg	823.04	J/mol×K	998.84	Joback Method

Sources

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=U321694&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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