«beta»-Alanine, N-(3-trifluoromethylbenzoyl)-, ethyl ester

Inchi: InChI=1S/C13H14F3NO3/c1-2-20-11(18)6-7-17-12(19)9-4-3-5-10(8-9)13(14,15)16/h3-5,8

InchiKey: NIJZVCCXQUNHIU-UHFFFAOYSA-N

Formula: C13H14F3NO3

SMILES: CCOC(=O)CCNC(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 289.25

Physical Properties

Property code	Value	Unit	Source
gf	-693.68	kJ/mol	Joback Method
hf	-987.58	kJ/mol	Joback Method
hfus	34.39	kJ/mol	Joback Method
hvap	66.06	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.388		Crippen Method
mcvol	194.570	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	1832.00		NIST Webbook
rinpol	1832.00		NIST Webbook
tb	703.41	K	Joback Method
tc	900.12	K	Joback Method
tf	454.15	K	Joback Method
vc	0.763	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.40	J/mol×K	703.41	Joback Method
cpg	552.76	J/mol×K	736.20	Joback Method
cpg	564.27	J/mol×K	768.98	Joback Method
cpg	574.97	J/mol×K	801.77	Joback Method
cpg	584.91	J/mol×K	834.55	Joback Method
cpg	594.10	J/mol×K	867.34	Joback Method
cpg	602.60	J/mol×K	900.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321584&Units=SI
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

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