

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

Inchi:	InChI=1S/C15H18F3NO3/c1-2-3-9-22-13(20)7-8-19-14(21)11-5-4-6-12(10-11)15(16,17)1
InchiKey:	RQWSSIQMHUEKSH-UHFFFAOYSA-N
Formula:	C15H18F3NO3
SMILES:	CCCCOC(=O)CCNC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]:	317.30

Physical Properties

Property code	Value	Unit	Source
gf	-676.84	kJ/mol	Joback Method
hf	-1028.86	kJ/mol	Joback Method
hfus	39.57	kJ/mol	Joback Method
hvap	70.51	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.169		Crippen Method
mcvol	222.750	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	2037.00		NIST Webbook
tb	749.17	K	Joback Method
tc	943.25	K	Joback Method
tf	476.69	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.88	J/molxK	749.17	Joback Method
cpg	660.04	J/molxK	781.52	Joback Method
cpg	672.31	J/molxK	813.86	Joback Method
cpg	683.73	J/molxK	846.21	Joback Method
cpg	694.36	J/molxK	878.55	Joback Method
cpg	704.21	J/molxK	910.90	Joback Method
cpg	713.35	J/molxK	943.25	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=U321586&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
mccvol:	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

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