

«beta»-Alanine, N-(4-trifluoromethylbenzoyl)-, ethyl ester

Inchi:	InChI=1S/C13H14F3NO3/c1-2-20-11(18)7-8-17-12(19)9-3-5-10(6-4-9)13(14,15)16/h3-6H
InchiKey:	BELQGTLEMRHCFH-UHFFFAOYSA-N
Formula:	C13H14F3NO3
SMILES:	CCOC(=O)CCNC(=O)c1ccc(C(F)(F)F)cc1
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	1823.00		NIST Webbook
rinpol	1823.00		NIST Webbook
tb	703.41	K	Joback Method
tc	900.12	K	Joback Method
tf	454.15	K	Joback Method
vc	0.763	m ³ /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=U321737&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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