Ethyl N-benzyl-N-(trifluoroacetyl)-«beta»-alaninate

Other names: Ethyl 3-(N-trifluoroacetyl-N-benzylamino)propanoate
Inchi: InChI=1S/C14H16F3NO3/c1-2-21-12(19)8-9-18(13(20)14(15,16)17)10-11-6-4-3-5-7-11/h
InchiKey: BXWPXTDJOKUPKS-UHFFFAOYSA-N
Formula: C14H16F3NO3
SMILES: CCOC(=O)CCN(Cc1ccccc1)C(=O)C(F)(F)F
Mol. weight [g/mol]: 303.28

Physical Properties

Property code	Value	Unit	Source
gf	-654.24	kJ/mol	Joback Method
hf	-982.69	kJ/mol	Joback Method
hfus	35.29	kJ/mol	Joback Method
hvap	63.23	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.531		Crippen Method
mcvol	208.660	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	1747.00		NIST Webbook
tb	683.58	K	Joback Method
tc	874.66	K	Joback Method
tf	432.71	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.73	J/mol×K	683.58	Joback Method
cpg	593.41	J/mol×K	715.43	Joback Method
cpg	606.18	J/mol×K	747.27	Joback Method
cpg	618.07	J/mol×K	779.12	Joback Method
cpg	629.14	J/mol×K	810.97	Joback Method
cpg	639.43	J/mol×K	842.81	Joback Method
cpg	648.99	J/mol×K	874.66	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=U373372&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
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