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

Inchi: InChI=1S/C19H26F3NO3/c1-2-3-4-5-6-7-14-26-17(24)12-13-23-18(25)15-8-10-16(11-9-1

InchiKey: CNTAVCPNKSHDDL-UHFFFAOYSA-N

Formula: C19H26F3NO3

SMILES: CCCCCCCCOC(=O)CCNC(=O)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 373.41

Physical Properties

Property code	Value	Unit	Source
gf	-643.16	kJ/mol	Joback Method
hf	-1111.42	kJ/mol	Joback Method
hfus	49.93	kJ/mol	Joback Method
hvap	79.42	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	4.729		Crippen Method
mcvol	279.110	ml/mol	McGowan Method
pc	1351.64	kPa	Joback Method
rinpol	2414.00		NIST Webbook
tb	840.69	K	Joback Method
tc	1036.30	K	Joback Method
tf	521.77	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.16	J/mol×K	840.69	Joback Method
cpg	886.65	J/mol×K	873.29	Joback Method
cpg	900.16	J/mol×K	905.89	Joback Method
cpg	912.73	J/mol×K	938.50	Joback Method
cpg	924.43	J/mol×K	971.10	Joback Method
cpg	935.29	J/mol×K	1003.70	Joback Method
cpg	945.38	J/mol×K	1036.30	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=U321742&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