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

Inchi: InChI=1S/C20H28F3NO3/c1-2-3-4-5-6-7-8-15-27-18(25)13-14-24-19(26)16-9-11-17(12-1

InchiKey: GRFHPRRDMSMPEX-UHFFFAOYSA-N

Formula: C20H28F3NO3

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

Mol. weight [g/mol]: 387.44

Physical Properties

Property code	Value	Unit	Source
gf	-634.74	kJ/mol	Joback Method
hf	-1132.06	kJ/mol	Joback Method
hfus	52.52	kJ/mol	Joback Method
hvap	81.64	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.119		Crippen Method
mcvol	293.200	ml/mol	McGowan Method
pc	1261.06	kPa	Joback Method
rinpol	2513.00		NIST Webbook
rinpol	2513.00		NIST Webbook
tb	863.57	K	Joback Method
tc	1061.28	K	Joback Method
tf	533.04	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	930.66	J/mol×K	863.57	Joback Method
cpg	945.48	J/mol×K	896.52	Joback Method
cpg	959.29	J/mol×K	929.47	Joback Method
cpg	972.14	J/mol×K	962.43	Joback Method
cpg	984.08	J/mol×K	995.38	Joback Method
cpg	995.18	J/mol×K	1028.33	Joback Method
cpg	1005.47	J/mol×K	1061.28	Joback Method

Sources

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=U321743&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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