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

Inchi: InChI=1S/C16H20F3NO3/c1-2-3-4-10-23-14(21)8-9-20-15(22)12-6-5-7-13(11-12)16(17,1

InchiKey: UBPLKQNAZPNFGL-UHFFFAOYSA-N

Formula: C16H20F3NO3

SMILES: CCCCCOC(=O)CCNC(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 331.33

Physical Properties

Property code	Value	Unit	Source
gf	-668.42	kJ/mol	Joback Method
hf	-1049.50	kJ/mol	Joback Method
hfus	42.16	kJ/mol	Joback Method
hvap	72.74	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.559		Crippen Method
mcvol	236.840	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	2137.00		NIST Webbook
rinpol	2137.00		NIST Webbook
tb	772.05	K	Joback Method
tc	965.59	K	Joback Method
tf	487.96	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.76	J/mol×K	772.05	Joback Method
cpg	715.27	J/mol×K	804.31	Joback Method
cpg	727.87	J/mol×K	836.56	Joback Method
cpg	739.61	J/mol×K	868.82	Joback Method
cpg	750.53	J/mol×K	901.07	Joback Method
cpg	760.67	J/mol×K	933.33	Joback Method
cpg	770.07	J/mol×K	965.59	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=U321587&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