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

Inchi: InChI=1S/C26H40F3NO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-20-33-24(31)18-19-30-25(3

InchiKey: UZSRVXIDJBYBOZ-UHFFFAOYSA-N

Formula: C26H40F3NO3

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

Mol. weight [g/mol]: 471.60

Physical Properties

Property code	Value	Unit	Source
gf	-584.22	kJ/mol	Joback Method
hf	-1255.90	kJ/mol	Joback Method
hfus	68.06	kJ/mol	Joback Method
hvap	95.00	kJ/mol	Joback Method
log10ws	-8.90		Crippen Method
logp	7.460		Crippen Method
mcvol	377.740	ml/mol	McGowan Method
pc	869.14	kPa	Joback Method
rinpol	3393.00		NIST Webbook
rinpol	3393.00		NIST Webbook
tb	1000.85	K	Joback Method
tc	1230.34	K	Joback Method
tf	600.66	K	Joback Method
vc	1.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1295.64	J/mol×K	1000.85	Joback Method
cpg	1313.14	J/mol×K	1039.10	Joback Method
cpg	1329.29	J/mol×K	1077.35	Joback Method
cpg	1344.19	J/mol×K	1115.59	Joback Method
cpg	1357.96	J/mol×K	1153.84	Joback Method
cpg	1370.71	J/mol×K	1192.09	Joback Method
cpg	1382.53	J/mol×K	1230.34	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=U321597&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