«beta»-Alanine, N-(2,3,4-trifluorobenzoyl)-, hexyl ester

Inchi: InChI=1S/C16H20F3NO3/c1-2-3-4-5-10-23-13(21)8-9-20-16(22)11-6-7-12(17)15(19)14(1

InchiKey: QNEOTFNETRZAHJ-UHFFFAOYSA-N

Formula: C16H20F3NO3

SMILES: CCCCCCOC(=O)CCNC(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 331.33

Physical Properties

Property code	Value	Unit	Source
gf	-690.52	kJ/mol	Joback Method
hf	-1063.69	kJ/mol	Joback Method
hfus	48.80	kJ/mol	Joback Method
hvap	75.36	kJ/mol	Joback Method
log10ws	-5.02		Crippen Method
logp	3.347		Crippen Method
mcvol	236.840	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	2154.00		NIST Webbook
rinpol	2154.00		NIST Webbook
tb	785.24	K	Joback Method
tc	974.99	K	Joback Method
tf	510.58	K	Joback Method
vc	0.943	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	697.93	J/mol×K	785.24	Joback Method
cpg	711.15	J/mol×K	816.87	Joback Method
cpg	723.55	J/mol×K	848.49	Joback Method
cpg	735.11	J/mol×K	880.12	Joback Method
cpg	745.88	J/mol×K	911.74	Joback Method
cpg	755.85	J/mol×K	943.37	Joback Method
cpg	765.04	J/mol×K	974.99	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=U321693&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

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