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

Inchi: InChI=1S/C18H24F3NO3/c1-2-3-4-5-6-13-25-16(23)11-12-22-17(24)14-7-9-15(10-8-14)1

InchiKey: OMTPASBBZVIDST-UHFFFAOYSA-N

Formula: C18H24F3NO3

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

Mol. weight [g/mol]: 359.38

Physical Properties

Property code	Value	Unit	Source
gf	-651.58	kJ/mol	Joback Method
hf	-1090.78	kJ/mol	Joback Method
hfus	47.34	kJ/mol	Joback Method
hvap	77.19	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.339		Crippen Method
mcvol	265.020	ml/mol	McGowan Method
pc	1452.35	kPa	Joback Method
rinpol	2314.00		NIST Webbook
rinpol	2314.00		NIST Webbook
tb	817.81	K	Joback Method
tc	1012.06	K	Joback Method
tf	510.50	K	Joback Method
vc	1.044	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.47	J/mol×K	817.81	Joback Method
cpg	828.63	J/mol×K	850.19	Joback Method
cpg	841.84	J/mol×K	882.56	Joback Method
cpg	854.15	J/mol×K	914.94	Joback Method
cpg	865.60	J/mol×K	947.31	Joback Method
cpg	876.23	J/mol×K	979.69	Joback Method
cpg	886.10	J/mol×K	1012.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321741&Units=SI
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

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