D-Alanine, N-(2,4,5-trifluoro-3-methoxybenzoyl)-, isohexyl ester

Inchi: InChI=1S/C17H22F3NO4/c1-9(2)6-5-7-25-17(23)10(3)21-16(22)11-8-12(18)14(20)15(24-

InchiKey: UAHKYLNPTOQFSJ-UHFFFAOYSA-N

Formula: C17H22F3NO4

SMILES: COc1c(F)c(F)cc(C(=O)NC(C)C(=O)OCCCC(C)C)c1F

Mol. weight [g/mol]: 361.36

Physical Properties

Property code	Value	Unit	Source
gf	-801.61	kJ/mol	Joback Method
hf	-1238.58	kJ/mol	Joback Method
hfus	45.14	kJ/mol	Joback Method
hvap	79.88	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	3.210		Crippen Method
mcvol	256.800	ml/mol	McGowan Method
pc	1487.29	kPa	Joback Method
rinpol	2224.00		NIST Webbook
tb	834.64	K	Joback Method
tc	1030.84	K	Joback Method
tf	526.60	K	Joback Method
vc	1.004	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	782.20	J/mol×K	834.64	Joback Method
cpg	795.63	J/mol×K	867.34	Joback Method
cpg	808.07	J/mol×K	900.04	Joback Method
cpg	819.50	J/mol×K	932.74	Joback Method
cpg	829.95	J/mol×K	965.44	Joback Method
cpg	839.40	J/mol×K	998.14	Joback Method
cpg	847.86	J/mol×K	1030.84	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=U348451&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