D-Alanine, N-(2-fluoro-5-trifluoromethylbenzoyl)-, propyl ester

Inchi: InChI=1S/C14H15F4NO3/c1-3-6-22-13(21)8(2)19-12(20)10-7-9(14(16,17)18)4-5-11(10)1

InchiKey: ZPKWQZNGGMKCNQ-UHFFFAOYSA-N

Formula: C14H15F4NO3

SMILES: CCCOC(=O)C(C)NC(=O)c1cc(C(F)(F)F)ccc1F

Mol. weight [g/mol]: 321.27

Physical Properties

Property code	Value	Unit	Source
gf	-892.14	kJ/mol	Joback Method
hf	-1221.08	kJ/mol	Joback Method
hfus	36.15	kJ/mol	Joback Method
hvap	67.74	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	2.916		Crippen Method
mcvol	210.430	ml/mol	McGowan Method
pc	1903.58	kPa	Joback Method
rinpol	1772.00		NIST Webbook
rinpol	1772.00		NIST Webbook
tb	730.10	K	Joback Method
tc	922.47	K	Joback Method
tf	463.53	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.40	J/mol×K	730.10	Joback Method
cpg	612.76	J/mol×K	762.16	Joback Method
cpg	624.30	J/mol×K	794.22	Joback Method
cpg	635.04	J/mol×K	826.29	Joback Method
cpg	645.01	J/mol×K	858.35	Joback Method
cpg	654.25	J/mol×K	890.41	Joback Method
cpg	662.78	J/mol×K	922.47	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=U348344&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