D-Alanine, N-(2-fluoro-3-trifluoromethylbenzoyl)-, isobutyl ester

Inchi: InChI=1S/C15H17F4NO3/c1-8(2)7-23-14(22)9(3)20-13(21)10-5-4-6-11(12(10)16)15(17,1

InchiKey: CPTACUVKBQHOBY-UHFFFAOYSA-N

Formula: C15H17F4NO3

SMILES: CC(C)COC(=O)C(C)NC(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 335.29

Physical Properties

Property code	Value	Unit	Source
gf	-886.16	kJ/mol	Joback Method
hf	-1247.00	kJ/mol	Joback Method
hfus	35.21	kJ/mol	Joback Method
hvap	69.58	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.162		Crippen Method
mcvol	224.520	ml/mol	McGowan Method
pc	1765.41	kPa	Joback Method
rinpol	1841.00		NIST Webbook
rinpol	1841.00		NIST Webbook
tb	752.54	K	Joback Method
tc	946.57	K	Joback Method
tf	459.80	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.74	J/mol×K	752.54	Joback Method
cpg	667.67	J/mol×K	784.88	Joback Method
cpg	679.72	J/mol×K	817.22	Joback Method
cpg	690.91	J/mol×K	849.55	Joback Method
cpg	701.29	J/mol×K	881.89	Joback Method
cpg	710.89	J/mol×K	914.23	Joback Method
cpg	719.75	J/mol×K	946.57	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=U348418&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