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

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

InchiKey: RTLBSEKRVXZCHS-UHFFFAOYSA-N

Formula: C15H17F4NO3

SMILES: CCCCOC(=O)C(C)NC(=O)c1cc(F)ccc1C(F)(F)F

Mol. weight [g/mol]: 335.29

Physical Properties

Property code	Value	Unit	Source
gf	-883.72	kJ/mol	Joback Method
hf	-1241.72	kJ/mol	Joback Method
hfus	38.74	kJ/mol	Joback Method
hvap	69.97	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.306		Crippen Method
mcvol	224.520	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	1868.00		NIST Webbook
tb	752.98	K	Joback Method
tc	944.62	K	Joback Method
tf	474.80	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.17	J/mol×K	752.98	Joback Method
cpg	666.93	J/mol×K	784.92	Joback Method
cpg	678.84	J/mol×K	816.86	Joback Method
cpg	689.93	J/mol×K	848.80	Joback Method
cpg	700.23	J/mol×K	880.74	Joback Method
cpg	709.78	J/mol×K	912.68	Joback Method
cpg	718.60	J/mol×K	944.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348432&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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