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

Inchi: InChI=1S/C13H13F4NO3/c1-3-21-12(20)7(2)18-11(19)9-6-8(13(15,16)17)4-5-10(9)14/h4
InchiKey: BOOVSODMISPVBW-UHFFFAOYSA-N
Formula: C13H13F4NO3
SMILES: CCOC(=O)C(C)NC(=O)c1cc(C(F)(F)F)ccc1F
Mol. weight [g/mol]: 307.24

Physical Properties

Property code	Value	Unit	Source
gf	-900.56	kJ/mol	Joback Method
hf	-1200.44	kJ/mol	Joback Method
hfus	33.56	kJ/mol	Joback Method
hvap	65.52	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	2.526		Crippen Method
mcvol	196.340	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	1681.00		NIST Webbook
rinpol	1681.00		NIST Webbook
tb	707.22	K	Joback Method
tc	900.82	K	Joback Method
tf	452.26	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	547.77	J/mol×K	707.22	Joback Method
cpg	559.70	J/mol×K	739.49	Joback Method
cpg	570.82	J/mol×K	771.75	Joback Method
cpg	581.17	J/mol×K	804.02	Joback Method
cpg	590.78	J/mol×K	836.29	Joback Method
cpg	599.67	J/mol×K	868.55	Joback Method
cpg	607.87	J/mol×K	900.82	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=U348343&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

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