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

Inchi: InChI=1S/C23H33F4NO3/c1-3-4-5-6-7-8-9-10-11-12-15-31-22(30)17(2)28-21(29)19-16-1
InchiKey: VGIIUFGNTVPDTC-UHFFFAOYSA-N
Formula: C23H33F4NO3
SMILES: CCCCCCCCCCCCOC(=O)C(C)NC(=O)c1cc(C(F)(F)F)ccc1F
Mol. weight [g/mol]: 447.51

Physical Properties

Property code	Value	Unit	Source
gf	-816.36	kJ/mol	Joback Method
hf	-1406.84	kJ/mol	Joback Method
hfus	59.46	kJ/mol	Joback Method
hvap	87.78	kJ/mol	Joback Method
log10ws	-8.09		Crippen Method
logp	6.427		Crippen Method
mcvol	337.240	ml/mol	McGowan Method
pc	1003.98	kPa	Joback Method
rinpol	2634.00		NIST Webbook
rinpol	2634.00		NIST Webbook
tb	936.02	K	Joback Method
tc	1146.12	K	Joback Method
tf	564.96	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1117.18	J/mol×K	936.02	Joback Method
cpg	1132.91	J/mol×K	971.04	Joback Method
cpg	1147.47	J/mol×K	1006.05	Joback Method
cpg	1160.92	J/mol×K	1041.07	Joback Method
cpg	1173.33	J/mol×K	1076.09	Joback Method
cpg	1184.77	J/mol×K	1111.10	Joback Method
cpg	1195.31	J/mol×K	1146.12	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=U348353&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