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

Inchi: InChI=1S/C21H29F4NO3/c1-3-4-5-6-7-8-9-10-14-29-20(28)15(2)26-19(27)16-12-11-13-1

InchiKey: BDWNAXYBTWMAEN-UHFFFAOYSA-N

Formula: C21H29F4NO3

SMILES: CCCCCCCCCCOC(=O)C(C)NC(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 419.45

Physical Properties

Property code	Value	Unit	Source
gf	-833.20	kJ/mol	Joback Method
hf	-1365.56	kJ/mol	Joback Method
hfus	54.28	kJ/mol	Joback Method
hvap	83.33	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	5.647		Crippen Method
mcvol	309.060	ml/mol	McGowan Method
pc	1138.27	kPa	Joback Method
rinpol	2461.00		NIST Webbook
tb	890.26	K	Joback Method
tc	1090.89	K	Joback Method
tf	542.42	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	996.83	J/mol×K	890.26	Joback Method
cpg	1011.74	J/mol×K	923.70	Joback Method
cpg	1025.58	J/mol×K	957.14	Joback Method
cpg	1038.41	J/mol×K	990.58	Joback Method
cpg	1050.29	J/mol×K	1024.02	Joback Method
cpg	1061.27	J/mol×K	1057.46	Joback Method
cpg	1071.41	J/mol×K	1090.89	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=U348421&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