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

Inchi: InChI=1S/C20H27F4NO3/c1-3-4-5-6-7-8-9-13-28-19(27)14(2)25-18(26)15-11-10-12-16(1

InchiKey: RDKLTVCHMFMEOQ-UHFFFAOYSA-N

Formula: C20H27F4NO3

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

Mol. weight [g/mol]: 405.43

Physical Properties

Property code	Value	Unit	Source
gf	-841.62	kJ/mol	Joback Method
hf	-1344.92	kJ/mol	Joback Method
hfus	51.69	kJ/mol	Joback Method
hvap	81.10	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	5.257		Crippen Method
mcvol	294.970	ml/mol	McGowan Method
pc	1215.74	kPa	Joback Method
rinpol	2360.00		NIST Webbook
rinpol	2360.00		NIST Webbook
tb	867.38	K	Joback Method
tc	1064.65	K	Joback Method
tf	531.15	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.66	J/mol×K	867.38	Joback Method
cpg	952.19	J/mol×K	900.26	Joback Method
cpg	965.71	J/mol×K	933.14	Joback Method
cpg	978.25	J/mol×K	966.02	Joback Method
cpg	989.88	J/mol×K	998.89	Joback Method
cpg	1000.64	J/mol×K	1031.77	Joback Method
cpg	1010.59	J/mol×K	1064.65	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348420&Units=SI

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