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

Inchi: InChI=1S/C19H25F4NO3/c1-3-4-5-6-7-8-12-27-18(26)13(2)24-17(25)14-10-9-11-15(16(1

InchiKey: XUAQAJLHQBJQOC-UHFFFAOYSA-N

Formula: C19H25F4NO3

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

Mol. weight [g/mol]: 391.40

Physical Properties

Property code	Value	Unit	Source
gf	-850.04	kJ/mol	Joback Method
hf	-1324.28	kJ/mol	Joback Method
hfus	49.10	kJ/mol	Joback Method
hvap	78.87	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	4.867		Crippen Method
mcvol	280.880	ml/mol	McGowan Method
pc	1301.41	kPa	Joback Method
rinpol	2261.00		NIST Webbook
tb	844.50	K	Joback Method
tc	1039.23	K	Joback Method
tf	519.88	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	879.24	J/mol×K	844.50	Joback Method
cpg	893.41	J/mol×K	876.96	Joback Method
cpg	906.61	J/mol×K	909.41	Joback Method
cpg	918.88	J/mol×K	941.87	Joback Method
cpg	930.26	J/mol×K	974.32	Joback Method
cpg	940.80	J/mol×K	1006.78	Joback Method
cpg	950.55	J/mol×K	1039.23	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348419&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

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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