D-Alanine, N-(3,4-difluorobenzoyl)-, octyl ester

Inchi: InChI=1S/C18H25F2NO3/c1-3-4-5-6-7-8-11-24-18(23)13(2)21-17(22)14-9-10-15(19)16(2
InchiKey: OSXWZAJWZWIYAP-UHFFFAOYSA-N
Formula: C18H25F2NO3
SMILES: CCCCCCCCOC(=O)C(C)NC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 341.39

Physical Properties

Property code	Value	Unit	Source
gf	-471.68	kJ/mol	Joback Method
hf	-902.67	kJ/mol	Joback Method
hfus	47.76	kJ/mol	Joback Method
hvap	79.58	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	3.987		Crippen Method
mcvol	263.250	ml/mol	McGowan Method
pc	1473.62	kPa	Joback Method
rinpol	2337.00		NIST Webbook
rinpol	2337.00		NIST Webbook
tb	826.31	K	Joback Method
tc	1022.60	K	Joback Method
tf	505.01	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.34	J/mol×K	826.31	Joback Method
cpg	819.86	J/mol×K	859.03	Joback Method
cpg	833.39	J/mol×K	891.74	Joback Method
cpg	845.97	J/mol×K	924.46	Joback Method
cpg	857.60	J/mol×K	957.17	Joback Method
cpg	868.33	J/mol×K	989.89	Joback Method
cpg	878.18	J/mol×K	1022.60	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=U348363&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