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

Inchi: InChI=1S/C20H29F2NO3/c1-3-4-5-6-7-8-9-10-13-26-20(25)15(2)23-19(24)16-11-12-17(2
InchiKey: MPFBRGDGWNYEIQ-UHFFFAOYSA-N
Formula: C20H29F2NO3
SMILES: CCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 369.45

Physical Properties

Property code	Value	Unit	Source
gf	-454.84	kJ/mol	Joback Method
hf	-943.95	kJ/mol	Joback Method
hfus	52.94	kJ/mol	Joback Method
hvap	84.03	kJ/mol	Joback Method
log10ws	-6.48		Crippen Method
logp	4.767		Crippen Method
mcvol	291.430	ml/mol	McGowan Method
pc	1278.25	kPa	Joback Method
rinpol	2532.00		NIST Webbook
rinpol	2532.00		NIST Webbook
tb	872.07	K	Joback Method
tc	1071.74	K	Joback Method
tf	527.55	K	Joback Method
vc	1.143	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	922.29	J/mol×K	872.07	Joback Method
cpg	937.42	J/mol×K	905.35	Joback Method
cpg	951.47	J/mol×K	938.63	Joback Method
cpg	964.47	J/mol×K	971.91	Joback Method
cpg	976.45	J/mol×K	1005.19	Joback Method
cpg	987.46	J/mol×K	1038.46	Joback Method
cpg	997.51	J/mol×K	1071.74	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=U348365&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