D-Alanine, N-(2,5-ditrifluoromethylbenzoyl)-, pentyl ester

Inchi: InChI=1S/C17H19F6NO3/c1-3-4-5-8-27-15(26)10(2)24-14(25)12-9-11(16(18,19)20)6-7-1

InchiKey: NVSYQQDCBWLBNS-UHFFFAOYSA-N

Formula: C17H19F6NO3

SMILES: CCCCCOC(=O)C(C)NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 399.33

Physical Properties

Property code	Value	Unit	Source
gf	-1253.66	kJ/mol	Joback Method
hf	-1683.97	kJ/mol	Joback Method
hfus	42.66	kJ/mol	Joback Method
hvap	71.49	kJ/mol	Joback Method
log10ws	-5.93		Crippen Method
logp	4.576		Crippen Method
mcvol	256.240	ml/mol	McGowan Method
pc	1422.92	kPa	Joback Method
rinpol	1876.00		NIST Webbook
tb	794.05	K	Joback Method
tc	982.43	K	Joback Method
tf	500.94	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.73	J/mol×K	794.05	Joback Method
cpg	794.54	J/mol×K	825.45	Joback Method
cpg	806.46	J/mol×K	856.84	Joback Method
cpg	817.55	J/mol×K	888.24	Joback Method
cpg	827.87	J/mol×K	919.64	Joback Method
cpg	837.46	J/mol×K	951.03	Joback Method
cpg	846.38	J/mol×K	982.43	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=U347800&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