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

Inchi: InChI=1S/C22H29F6NO3/c1-3-4-5-6-7-8-9-10-13-32-20(31)15(2)29-19(30)17-14-16(21(2
InchiKey: SYDKYAMEEMVKRS-UHFFFAOYSA-N
Formula: C22H29F6NO3
SMILES: CCCCCCCCCCOC(=O)C(C)NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 469.46

Physical Properties

Property code	Value	Unit	Source
gf	-1211.56	kJ/mol	Joback Method
hf	-1787.17	kJ/mol	Joback Method
hfus	55.61	kJ/mol	Joback Method
hvap	82.62	kJ/mol	Joback Method
log10ws	-8.02		Crippen Method
logp	6.526		Crippen Method
mcvol	326.690	ml/mol	McGowan Method
pc	1020.08	kPa	Joback Method
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
tb	908.45	K	Joback Method
tc	1112.20	K	Joback Method
tf	557.29	K	Joback Method
vc	1.304	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1071.38	J/mol×K	908.45	Joback Method
cpg	1086.22	J/mol×K	942.41	Joback Method
cpg	1100.02	J/mol×K	976.37	Joback Method
cpg	1112.86	J/mol×K	1010.33	Joback Method
cpg	1124.81	J/mol×K	1044.29	Joback Method
cpg	1135.96	J/mol×K	1078.24	Joback Method
cpg	1146.40	J/mol×K	1112.20	Joback Method

Sources

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=U347805&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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