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

Inchi: InChI=1S/C14H13F6NO3/c1-3-24-12(23)7(2)21-11(22)9-6-8(13(15,16)17)4-5-10(9)14(18

InchiKey: HCESQNKXWSKSND-UHFFFAOYSA-N

Formula: C14H13F6NO3

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

Mol. weight [g/mol]: 357.25

Physical Properties

Property code	Value	Unit	Source
gf	-1278.92	kJ/mol	Joback Method
hf	-1622.05	kJ/mol	Joback Method
hfus	34.89	kJ/mol	Joback Method
hvap	64.81	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.406		Crippen Method
mcvol	213.970	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	1517.00		NIST Webbook
rinpol	1517.00		NIST Webbook
tb	725.41	K	Joback Method
tc	912.99	K	Joback Method
tf	467.13	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.66	J/mol×K	725.41	Joback Method
cpg	630.32	J/mol×K	756.67	Joback Method
cpg	641.16	J/mol×K	787.94	Joback Method
cpg	651.21	J/mol×K	819.20	Joback Method
cpg	660.53	J/mol×K	850.46	Joback Method
cpg	669.15	J/mol×K	881.72	Joback Method
cpg	677.13	J/mol×K	912.99	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=U347797&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