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

Inchi: InChI=1S/C15H15F6NO3/c1-3-6-25-13(24)8(2)22-12(23)10-7-9(14(16,17)18)4-5-11(10)1

InchiKey: MMUIISYGDAKMDQ-UHFFFAOYSA-N

Formula: C15H15F6NO3

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

Mol. weight [g/mol]: 371.27

Physical Properties

Property code	Value	Unit	Source
gf	-1270.50	kJ/mol	Joback Method
hf	-1642.69	kJ/mol	Joback Method
hfus	37.48	kJ/mol	Joback Method
hvap	67.04	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	3.796		Crippen Method
mcvol	228.060	ml/mol	McGowan Method
pc	1653.80	kPa	Joback Method
rinpol	1693.00		NIST Webbook
tb	748.29	K	Joback Method
tc	935.56	K	Joback Method
tf	478.40	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.98	J/mol×K	748.29	Joback Method
cpg	684.04	J/mol×K	779.50	Joback Method
cpg	695.25	J/mol×K	810.71	Joback Method
cpg	705.67	J/mol×K	841.93	Joback Method
cpg	715.34	J/mol×K	873.14	Joback Method
cpg	724.31	J/mol×K	904.35	Joback Method
cpg	732.62	J/mol×K	935.56	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=U347798&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