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

Inchi: InChI=1S/C19H23F6NO3/c1-3-4-5-6-7-10-29-17(28)12(2)26-16(27)14-11-13(18(20,21)22
InchiKey: GJYLWXNMGLETHJ-UHFFFAOYSA-N
Formula: C19H23F6NO3
SMILES: CCCCCCCOC(=O)C(C)NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 427.38

Physical Properties

Property code	Value	Unit	Source
gf	-1236.82	kJ/mol	Joback Method
hf	-1725.25	kJ/mol	Joback Method
hfus	47.84	kJ/mol	Joback Method
hvap	75.94	kJ/mol	Joback Method
log10ws	-6.77		Crippen Method
logp	5.356		Crippen Method
mcvol	284.420	ml/mol	McGowan Method
pc	1237.22	kPa	Joback Method
rinpol	2052.00		NIST Webbook
rinpol	2052.00		NIST Webbook
tb	839.81	K	Joback Method
tc	1031.94	K	Joback Method
tf	523.48	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	895.20	J/mol×K	839.81	Joback Method
cpg	908.76	J/mol×K	871.83	Joback Method
cpg	921.38	J/mol×K	903.85	Joback Method
cpg	933.13	J/mol×K	935.88	Joback Method
cpg	944.06	J/mol×K	967.90	Joback Method
cpg	954.25	J/mol×K	999.92	Joback Method
cpg	963.75	J/mol×K	1031.94	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=U347802&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