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

Inchi: InChI=1S/C20H25F6NO3/c1-3-4-5-6-7-8-11-30-18(29)13(2)27-17(28)15-12-14(19(21,22)
InchiKey: LESOGZVKAKFFCK-UHFFFAOYSA-N
Formula: C20H25F6NO3
SMILES: CCCCCCCCOC(=O)C(C)NC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F
Mol. weight [g/mol]: 441.41

Physical Properties

Property code	Value	Unit	Source
gf	-1228.40	kJ/mol	Joback Method
hf	-1745.89	kJ/mol	Joback Method
hfus	50.43	kJ/mol	Joback Method
hvap	78.17	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	5.746		Crippen Method
mcvol	298.510	ml/mol	McGowan Method
pc	1157.71	kPa	Joback Method
rinpol	2135.00		NIST Webbook
tb	862.69	K	Joback Method
tc	1057.83	K	Joback Method
tf	534.75	K	Joback Method
vc	1.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	953.18	J/mol×K	862.69	Joback Method
cpg	967.14	J/mol×K	895.21	Joback Method
cpg	980.13	J/mol×K	927.74	Joback Method
cpg	992.22	J/mol×K	960.26	Joback Method
cpg	1003.48	J/mol×K	992.79	Joback Method
cpg	1013.97	J/mol×K	1025.31	Joback Method
cpg	1023.76	J/mol×K	1057.83	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=U347803&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