D-Alanine, N-(4-fluoro-2-trifluoromethylbenzoyl)-, heptyl ester

Inchi: InChI=1S/C18H23F4NO3/c1-3-4-5-6-7-10-26-17(25)12(2)23-16(24)14-9-8-13(19)11-15(1

InchiKey: KIQJGUIUWRDKSY-UHFFFAOYSA-N

Formula: C18H23F4NO3

SMILES: CCCCCCCOC(=O)C(C)NC(=O)c1ccc(F)cc1C(F)(F)F

Mol. weight [g/mol]: 377.37

Physical Properties

Property code	Value	Unit	Source
gf	-858.46	kJ/mol	Joback Method
hf	-1303.64	kJ/mol	Joback Method
hfus	46.51	kJ/mol	Joback Method
hvap	76.65	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	4.476		Crippen Method
mcvol	266.790	ml/mol	McGowan Method
pc	1396.46	kPa	Joback Method
rinpol	2145.00		NIST Webbook
tb	821.62	K	Joback Method
tc	1014.57	K	Joback Method
tf	508.61	K	Joback Method
vc	1.056	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.61	J/mol×K	821.62	Joback Method
cpg	835.44	J/mol×K	853.78	Joback Method
cpg	848.33	J/mol×K	885.94	Joback Method
cpg	860.32	J/mol×K	918.10	Joback Method
cpg	871.45	J/mol×K	950.26	Joback Method
cpg	881.77	J/mol×K	982.42	Joback Method
cpg	891.31	J/mol×K	1014.57	Joback Method

Sources

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=U348404&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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