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

Inchi: InChI=1S/C16H19F4NO3/c1-3-4-5-8-24-15(23)10(2)21-14(22)12-7-6-11(17)9-13(12)16(1

InchiKey: SUQSFYGYILRTPR-UHFFFAOYSA-N

Formula: C16H19F4NO3

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

Mol. weight [g/mol]: 349.32

Physical Properties

Property code	Value	Unit	Source
gf	-875.30	kJ/mol	Joback Method
hf	-1262.36	kJ/mol	Joback Method
hfus	41.33	kJ/mol	Joback Method
hvap	72.20	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	3.696		Crippen Method
mcvol	238.610	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook
tb	775.86	K	Joback Method
tc	967.32	K	Joback Method
tf	486.07	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.01	J/mol×K	775.86	Joback Method
cpg	722.14	J/mol×K	807.77	Joback Method
cpg	734.40	J/mol×K	839.68	Joback Method
cpg	745.80	J/mol×K	871.59	Joback Method
cpg	756.40	J/mol×K	903.50	Joback Method
cpg	766.23	J/mol×K	935.41	Joback Method
cpg	775.31	J/mol×K	967.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348403&Units=SI
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

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