D-Alanine, N-(5-fluoro-2-trifluoromethylbenzoyl)-, hexyl ester

Inchi: InChI=1S/C17H21F4NO3/c1-3-4-5-6-9-25-16(24)11(2)22-15(23)13-10-12(18)7-8-14(13)1

InchiKey: UWVCZOXDQXZNBC-UHFFFAOYSA-N

Formula: C17H21F4NO3

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

Mol. weight [g/mol]: 363.35

Physical Properties

Property code	Value	Unit	Source
gf	-866.88	kJ/mol	Joback Method
hf	-1283.00	kJ/mol	Joback Method
hfus	43.92	kJ/mol	Joback Method
hvap	74.42	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.086		Crippen Method
mcvol	252.700	ml/mol	McGowan Method
pc	1502.31	kPa	Joback Method
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook
tb	798.74	K	Joback Method
tc	990.62	K	Joback Method
tf	497.34	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.85	J/mol×K	798.74	Joback Method
cpg	778.33	J/mol×K	830.72	Joback Method
cpg	790.91	J/mol×K	862.70	Joback Method
cpg	802.61	J/mol×K	894.68	Joback Method
cpg	813.49	J/mol×K	926.66	Joback Method
cpg	823.56	J/mol×K	958.64	Joback Method
cpg	832.89	J/mol×K	990.62	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=U348434&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