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

Inchi: InChI=1S/C26H39F4NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-34-25(33)20(2)31-24(3
InchiKey: NPQYVNUBKYWUCM-UHFFFAOYSA-N
Formula: C26H39F4NO3
SMILES: CCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(F)cc1C(F)(F)F
Mol. weight [g/mol]: 489.59

Physical Properties

Property code	Value	Unit	Source
gf	-791.10	kJ/mol	Joback Method
hf	-1468.76	kJ/mol	Joback Method
hfus	67.23	kJ/mol	Joback Method
hvap	94.46	kJ/mol	Joback Method
log10ws	-9.34		Crippen Method
logp	7.597		Crippen Method
mcvol	379.510	ml/mol	McGowan Method
pc	843.09	kPa	Joback Method
rinpol	2955.00		NIST Webbook
rinpol	2955.00		NIST Webbook
tb	1004.66	K	Joback Method
tc	1236.91	K	Joback Method
tf	598.77	K	Joback Method
vc	1.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1301.99	J/mol×K	1004.66	Joback Method
cpg	1319.28	J/mol×K	1043.37	Joback Method
cpg	1335.16	J/mol×K	1082.08	Joback Method
cpg	1349.72	J/mol×K	1120.78	Joback Method
cpg	1363.09	J/mol×K	1159.49	Joback Method
cpg	1375.35	J/mol×K	1198.20	Joback Method
cpg	1386.62	J/mol×K	1236.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348412&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