

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

InChI: InChI=1S/C27H41F4NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-35-26(34)21(2)32-2
InChIKey: AX1DXHHCTXMBIH-UHFFFAOYSA-N

Formula: C27H41F4NO3

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

Mol. weight [g/mol]: 503.61

Physical Properties

Property code	Value	Unit	Source
gf	-782.68	kJ/mol	Joback Method
hf	-1489.40	kJ/mol	Joback Method
hfus	69.82	kJ/mol	Joback Method
hvap	96.68	kJ/mol	Joback Method
log10ws	-9.76		Crippen Method
logp	7.987		Crippen Method
mvol	393.600	ml/mol	McGowan Method
pc	797.98	kPa	Joback Method
rinpol	3040.00		NIST Webbook
rinpol	3040.00		NIST Webbook
tb	1027.54	K	Joback Method
tc	1269.63	K	Joback Method
tf	610.04	K	Joback Method
vc	1.560	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1364.57	J/molxK	1027.54	Joback Method
cpg	1382.49	J/molxK	1067.89	Joback Method
cpg	1398.90	J/molxK	1108.24	Joback Method
cpg	1413.91	J/molxK	1148.58	Joback Method
cpg	1427.65	J/molxK	1188.93	Joback Method
cpg	1440.25	J/molxK	1229.28	Joback Method
cpg	1451.83	J/molxK	1269.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348444&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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