

«beta»-Alanine, N-(4-fluorobenzoyl)-, tetradecyl ester

Inchi:	InChI=1S/C24H38FNO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-20-29-23(27)18-19-26-24(28)21
InchiKey:	RSLUVXDXHMZISR-UHFFFAOYSA-N
Formula:	C24H38FNO3
SMILES:	CCCCCCCCCCCCCOC(=O)CCNC(=O)c1ccc(F)cc1
Mol. weight [g/mol]:	407.56

Physical Properties

Property code	Value	Unit	Source
gf	-214.28	kJ/mol	Joback Method
hf	-813.65	kJ/mol	Joback Method
hfus	64.13	kJ/mol	Joback Method
hvap	93.48	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	6.190		Crippen Method
mvol	346.020	ml/mol	McGowan Method
pc	1021.38	kPa	Joback Method
rinpol	3273.00		NIST Webbook
rinpol	3273.00		NIST Webbook
tb	959.78	K	Joback Method
tc	1175.18	K	Joback Method
tf	574.52	K	Joback Method
vc	1.355	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1157.76	J/molxK	959.78	Joback Method
cpg	1174.52	J/molxK	995.68	Joback Method
cpg	1189.96	J/molxK	1031.58	Joback Method
cpg	1204.14	J/molxK	1067.48	Joback Method
cpg	1217.13	J/molxK	1103.38	Joback Method
cpg	1228.99	J/molxK	1139.28	Joback Method
cpg	1239.77	J/molxK	1175.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321765&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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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