

«beta»-Alanine, N-(3-fluorobenzoyl)-, nonyl ester

Inchi: InChI=1S/C19H28FNO3/c1-2-3-4-5-6-7-8-14-24-18(22)12-13-21-19(23)16-10-9-11-17(20)
InchiKey: NBZFYWQPOLTQHM-UHFFFAOYSA-N
Formula: C19H28FNO3
SMILES: CCCCCCCCCOC(=O)CCNC(=O)c1cccc(F)c1
Mol. weight [g/mol]: 337.43

Physical Properties

Property code	Value	Unit	Source
gf	-256.38	kJ/mol	Joback Method
hf	-710.45	kJ/mol	Joback Method
hfus	51.18	kJ/mol	Joback Method
hvap	82.35	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.239		Crippen Method
mcvol	275.570	ml/mol	McGowan Method
pc	1425.07	kPa	Joback Method
rinpol	2548.00		NIST Webbook
rinpol	2548.00		NIST Webbook
tb	845.38	K	Joback Method
tc	1044.13	K	Joback Method
tf	518.17	K	Joback Method
vc	1.075	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.31	J/mol×K	845.38	Joback Method
cpg	871.48	J/mol×K	878.51	Joback Method
cpg	885.61	J/mol×K	911.63	Joback Method
cpg	898.73	J/mol×K	944.76	Joback Method
cpg	910.89	J/mol×K	977.88	Joback Method
cpg	922.12	J/mol×K	1011.01	Joback Method
cpg	932.45	J/mol×K	1044.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321939&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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