Sarcosine, N-(2-fluorobenzoyl)-, butyl ester

Inchi: InChI=1S/C14H18FNO3/c1-3-4-9-19-13(17)10-16(2)14(18)11-7-5-6-8-12(11)15/h5-8H,3-

InchiKey: KARWYRRQPLZMBN-UHFFFAOYSA-N

Formula: C14H18FNO3

SMILES: CCCCOC(=O)CN(C)C(=O)c1ccccc1F

Mol. weight [g/mol]: 267.30

Physical Properties

Property code	Value	Unit	Source
gf	-277.09	kJ/mol	Joback Method
hf	-593.19	kJ/mol	Joback Method
hfus	36.15	kJ/mol	Joback Method
hvap	66.82	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.241		Crippen Method
mcvol	205.120	ml/mol	McGowan Method
pc	2096.50	kPa	Joback Method
rinpol	1962.00		NIST Webbook
rinpol	1962.00		NIST Webbook
tb	693.25	K	Joback Method
tc	890.84	K	Joback Method
tf	441.63	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.34	J/mol×K	693.25	Joback Method
cpg	574.62	J/mol×K	726.18	Joback Method
cpg	588.02	J/mol×K	759.11	Joback Method
cpg	600.56	J/mol×K	792.05	Joback Method
cpg	612.27	J/mol×K	824.98	Joback Method
cpg	623.18	J/mol×K	857.91	Joback Method
cpg	633.31	J/mol×K	890.84	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321242&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume