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

Inchi: InChI=1S/C14H18FNO3/c1-10(2)9-19-13(17)8-16(3)14(18)11-6-4-5-7-12(11)15/h4-7,10H
InchiKey: JNZGOBFCJDTKBT-UHFFFAOYSA-N
Formula: C14H18FNO3
SMILES: CC(C)COC(=O)CN(C)C(=O)c1ccccc1F
Mol. weight [g/mol]: 267.30

Physical Properties

Property code	Value	Unit	Source
gf	-279.53	kJ/mol	Joback Method
hf	-598.47	kJ/mol	Joback Method
hfus	32.63	kJ/mol	Joback Method
hvap	66.44	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	2.097		Crippen Method
mcvol	205.120	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	1914.00		NIST Webbook
rinpol	1914.00		NIST Webbook
tb	692.81	K	Joback Method
tc	893.63	K	Joback Method
tf	426.63	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.86	J/mol×K	692.81	Joback Method
cpg	575.40	J/mol×K	726.28	Joback Method
cpg	589.02	J/mol×K	759.75	Joback Method
cpg	601.74	J/mol×K	793.22	Joback Method
cpg	613.60	J/mol×K	826.69	Joback Method
cpg	624.62	J/mol×K	860.16	Joback Method
cpg	634.83	J/mol×K	893.63	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321241&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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