Sarcosine, N-(3-fluorobenzoyl)-, pentyl ester

Inchi: InChI=1S/C15H20FNO3/c1-3-4-5-9-20-14(18)11-17(2)15(19)12-7-6-8-13(16)10-12/h6-8,1
InchiKey: MZFQJMQKRBRTEM-UHFFFAOYSA-N
Formula: C15H20FNO3
SMILES: CCCCCOC(=O)CN(C)C(=O)c1cccc(F)c1
Mol. weight [g/mol]: 281.32

Physical Properties

Property code	Value	Unit	Source
gf	-268.67	kJ/mol	Joback Method
hf	-613.83	kJ/mol	Joback Method
hfus	38.74	kJ/mol	Joback Method
hvap	69.05	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.631		Crippen Method
mcvol	219.210	ml/mol	McGowan Method
pc	1923.67	kPa	Joback Method
rinpol	2059.00		NIST Webbook
rinpol	2059.00		NIST Webbook
tb	716.13	K	Joback Method
tc	911.96	K	Joback Method
tf	452.90	K	Joback Method
vc	0.834	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.95	J/mol×K	716.13	Joback Method
cpg	628.62	J/mol×K	748.77	Joback Method
cpg	642.38	J/mol×K	781.41	Joback Method
cpg	655.27	J/mol×K	814.05	Joback Method
cpg	667.30	J/mol×K	846.68	Joback Method
cpg	678.50	J/mol×K	879.32	Joback Method
cpg	688.92	J/mol×K	911.96	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=U321387&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