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

Inchi: InChI=1S/C16H22FNO3/c1-3-4-5-8-11-21-15(19)12-18(2)16(20)13-9-6-7-10-14(13)17/h6
InchiKey: BLGRJUVGYDKYIW-UHFFFAOYSA-N
Formula: C16H22FNO3
SMILES: CCCCCCOC(=O)CN(C)C(=O)c1ccccc1F
Mol. weight [g/mol]: 295.35

Physical Properties

Property code	Value	Unit	Source
gf	-260.25	kJ/mol	Joback Method
hf	-634.47	kJ/mol	Joback Method
hfus	41.34	kJ/mol	Joback Method
hvap	71.28	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.021		Crippen Method
mcvol	233.300	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	2157.00		NIST Webbook
tb	739.01	K	Joback Method
tc	933.54	K	Joback Method
tf	464.17	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.72	J/mol×K	739.01	Joback Method
cpg	683.74	J/mol×K	771.43	Joback Method
cpg	697.82	J/mol×K	803.85	Joback Method
cpg	711.00	J/mol×K	836.28	Joback Method
cpg	723.31	J/mol×K	868.70	Joback Method
cpg	734.77	J/mol×K	901.12	Joback Method
cpg	745.43	J/mol×K	933.54	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=U321245&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