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

Inchi: InChI=1S/C18H26FNO3/c1-3-4-5-6-7-10-13-23-17(21)14-20(2)18(22)15-11-8-9-12-16(15
InchiKey: OMFLLGHOEGMUPS-UHFFFAOYSA-N
Formula: C18H26FNO3
SMILES: CCCCCCCCOC(=O)CN(C)C(=O)c1ccccc1F
Mol. weight [g/mol]: 323.40

Physical Properties

Property code	Value	Unit	Source
gf	-243.41	kJ/mol	Joback Method
hf	-675.75	kJ/mol	Joback Method
hfus	46.51	kJ/mol	Joback Method
hvap	75.73	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.801		Crippen Method
mcvol	261.480	ml/mol	McGowan Method
pc	1516.39	kPa	Joback Method
rinpol	2367.00		NIST Webbook
rinpol	2367.00		NIST Webbook
tb	784.77	K	Joback Method
tc	978.29	K	Joback Method
tf	486.71	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	781.43	J/mol×K	784.77	Joback Method
cpg	797.05	J/mol×K	817.02	Joback Method
cpg	811.69	J/mol×K	849.28	Joback Method
cpg	825.37	J/mol×K	881.53	Joback Method
cpg	838.14	J/mol×K	913.78	Joback Method
cpg	850.03	J/mol×K	946.03	Joback Method
cpg	861.07	J/mol×K	978.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321246&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

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

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