Sarcosine, N-(2,6-difluorobenzoyl)-, hexyl ester

Inchi: InChI=1S/C16H21F2NO3/c1-3-4-5-6-10-22-14(20)11-19(2)16(21)15-12(17)8-7-9-13(15)1

InchiKey: SRHPYGIFPZVALH-UHFFFAOYSA-N

Formula: C16H21F2NO3

SMILES: CCCCCCOC(=O)CN(C)C(=O)c1c(F)cccc1F

Mol. weight [g/mol]: 313.34

Physical Properties

Property code	Value	Unit	Source
gf	-464.69	kJ/mol	Joback Method
hf	-842.05	kJ/mol	Joback Method
hfus	44.03	kJ/mol	Joback Method
hvap	71.12	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.160		Crippen Method
mcvol	235.070	ml/mol	McGowan Method
pc	1685.18	kPa	Joback Method
rinpol	2200.00		NIST Webbook
tb	743.26	K	Joback Method
tc	932.82	K	Joback Method
tf	477.28	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.73	J/mol×K	743.26	Joback Method
cpg	690.12	J/mol×K	774.85	Joback Method
cpg	703.64	J/mol×K	806.45	Joback Method
cpg	716.32	J/mol×K	838.04	Joback Method
cpg	728.17	J/mol×K	869.64	Joback Method
cpg	739.22	J/mol×K	901.23	Joback Method
cpg	749.49	J/mol×K	932.82	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321296&Units=SI

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