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

Inchi: InChI=1S/C15H19F2NO3/c1-3-4-5-9-21-13(19)10-18(2)15(20)14-11(16)7-6-8-12(14)17/h

InchiKey: BBOGTSLDJIVWGL-UHFFFAOYSA-N

Formula: C15H19F2NO3

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

Mol. weight [g/mol]: 299.31

Physical Properties

Property code	Value	Unit	Source
gf	-473.11	kJ/mol	Joback Method
hf	-821.41	kJ/mol	Joback Method
hfus	41.44	kJ/mol	Joback Method
hvap	68.89	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	2.770		Crippen Method
mcvol	220.980	ml/mol	McGowan Method
pc	1826.28	kPa	Joback Method
rinpol	2103.00		NIST Webbook
rinpol	2103.00		NIST Webbook
tb	720.38	K	Joback Method
tc	910.63	K	Joback Method
tf	466.01	K	Joback Method
vc	0.852	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.00	J/mol×K	720.38	Joback Method
cpg	635.01	J/mol×K	752.09	Joback Method
cpg	648.18	J/mol×K	783.80	Joback Method
cpg	660.52	J/mol×K	815.51	Joback Method
cpg	672.07	J/mol×K	847.21	Joback Method
cpg	682.85	J/mol×K	878.92	Joback Method
cpg	692.88	J/mol×K	910.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321295&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