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

Inchi: InChI=1S/C17H23F2NO3/c1-3-4-5-6-7-11-23-15(21)12-20(2)17(22)16-13(18)9-8-10-14(1

InchiKey: DLBCEPFXWZARMX-UHFFFAOYSA-N

Formula: C17H23F2NO3

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

Mol. weight [g/mol]: 327.37

Physical Properties

Property code	Value	Unit	Source
gf	-456.27	kJ/mol	Joback Method
hf	-862.69	kJ/mol	Joback Method
hfus	46.62	kJ/mol	Joback Method
hvap	73.35	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.550		Crippen Method
mcvol	249.160	ml/mol	McGowan Method
pc	1559.81	kPa	Joback Method
rinpol	2310.00		NIST Webbook
rinpol	2310.00		NIST Webbook
tb	766.14	K	Joback Method
tc	955.55	K	Joback Method
tf	488.55	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.54	J/mol×K	766.14	Joback Method
cpg	746.29	J/mol×K	797.71	Joback Method
cpg	760.13	J/mol×K	829.28	Joback Method
cpg	773.10	J/mol×K	860.85	Joback Method
cpg	785.22	J/mol×K	892.42	Joback Method
cpg	796.51	J/mol×K	923.99	Joback Method
cpg	807.00	J/mol×K	955.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321297&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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