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

Inchi: InChI=1S/C18H25F2NO3/c1-3-4-5-6-7-8-12-24-16(22)13-21(2)18(23)17-14(19)10-9-11-1
InchiKey: WQEWYHWFFHRMOP-UHFFFAOYSA-N
Formula: C18H25F2NO3
SMILES: CCCCCCCCOC(=O)CN(C)C(=O)c1c(F)cccc1F
Mol. weight [g/mol]: 341.39

Physical Properties

Property code	Value	Unit	Source
gf	-447.85	kJ/mol	Joback Method
hf	-883.33	kJ/mol	Joback Method
hfus	49.21	kJ/mol	Joback Method
hvap	75.57	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	3.940		Crippen Method
mcvol	263.250	ml/mol	McGowan Method
pc	1447.94	kPa	Joback Method
rinpol	2416.00		NIST Webbook
rinpol	2416.00		NIST Webbook
tb	789.02	K	Joback Method
tc	978.87	K	Joback Method
tf	499.82	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	788.35	J/mol×K	789.02	Joback Method
cpg	803.44	J/mol×K	820.66	Joback Method
cpg	817.59	J/mol×K	852.30	Joback Method
cpg	830.83	J/mol×K	883.94	Joback Method
cpg	843.18	J/mol×K	915.59	Joback Method
cpg	854.69	J/mol×K	947.23	Joback Method
cpg	865.38	J/mol×K	978.87	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=U321298&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