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

Inchi: InChI=1S/C20H29F2NO3/c1-3-4-5-6-7-8-9-10-14-26-18(24)15-23(2)20(25)19-16(21)12-1

InchiKey: UXGQDCDYVBEVGD-UHFFFAOYSA-N

Formula: C20H29F2NO3

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

Mol. weight [g/mol]: 369.45

Physical Properties

Property code	Value	Unit	Source
gf	-431.01	kJ/mol	Joback Method
hf	-924.61	kJ/mol	Joback Method
hfus	54.39	kJ/mol	Joback Method
hvap	80.02	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.721		Crippen Method
mcvol	291.430	ml/mol	McGowan Method
pc	1257.48	kPa	Joback Method
rinpol	2618.00		NIST Webbook
rinpol	2618.00		NIST Webbook
tb	834.78	K	Joback Method
tc	1027.47	K	Joback Method
tf	522.36	K	Joback Method
vc	1.131	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.68	J/mol×K	834.78	Joback Method
cpg	920.44	J/mol×K	866.89	Joback Method
cpg	935.17	J/mol×K	899.01	Joback Method
cpg	948.92	J/mol×K	931.12	Joback Method
cpg	961.72	J/mol×K	963.24	Joback Method
cpg	973.60	J/mol×K	995.35	Joback Method
cpg	984.61	J/mol×K	1027.47	Joback Method

Sources

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=U321300&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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