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

Inchi: InChI=1S/C25H39F2NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-19-31-23(29)20-28(2)25(3

InchiKey: SDTQVJRLDZFWHF-UHFFFAOYSA-N

Formula: C25H39F2NO3

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

Mol. weight [g/mol]: 439.58

Physical Properties

Property code	Value	Unit	Source
gf	-388.91	kJ/mol	Joback Method
hf	-1027.81	kJ/mol	Joback Method
hfus	67.34	kJ/mol	Joback Method
hvap	91.15	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	6.671		Crippen Method
mcvol	361.880	ml/mol	McGowan Method
pc	918.27	kPa	Joback Method
tb	949.18	K	Joback Method
tc	1163.23	K	Joback Method
tf	578.71	K	Joback Method
vc	1.411	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1208.37	J/mol×K	949.18	Joback Method
cpg	1226.09	J/mol×K	984.85	Joback Method
cpg	1242.47	J/mol×K	1020.53	Joback Method
cpg	1257.57	J/mol×K	1056.20	Joback Method
cpg	1271.45	J/mol×K	1091.88	Joback Method
cpg	1284.18	J/mol×K	1127.55	Joback Method
cpg	1295.83	J/mol×K	1163.23	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=U321304&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume