Sarcosine, n-pentafluorobenzoyl-, dodecyl ester

Inchi: InChI=1S/C22H30F5NO3/c1-3-4-5-6-7-8-9-10-11-12-13-31-15(29)14-28(2)22(30)16-17(2

InchiKey: DUPNDXBNTXNZHD-UHFFFAOYSA-N

Formula: C22H30F5NO3

SMILES: CCCCCCCCCCCCOC(=O)CN(C)C(=O)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 451.47

Physical Properties

Property code	Value	Unit	Source
gf	-1027.49	kJ/mol	Joback Method
hf	-1588.63	kJ/mol	Joback Method
hfus	67.64	kJ/mol	Joback Method
hvap	84.01	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	5.918		Crippen Method
mcvol	324.920	ml/mol	McGowan Method
pc	981.46	kPa	Joback Method
rinpol	2558.00		NIST Webbook
rinpol	2558.00		NIST Webbook
tb	893.29	K	Joback Method
tc	1094.38	K	Joback Method
tf	584.23	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1043.97	J/mol×K	893.29	Joback Method
cpg	1059.84	J/mol×K	926.80	Joback Method
cpg	1074.55	J/mol×K	960.32	Joback Method
cpg	1088.14	J/mol×K	993.83	Joback Method
cpg	1100.64	J/mol×K	1027.35	Joback Method
cpg	1112.08	J/mol×K	1060.86	Joback Method
cpg	1122.50	J/mol×K	1094.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321553&Units=SI

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