Sarcosine, n-pentafluorobenzoyl-, butyl ester

Inchi: InChI=1S/C14H14F5NO3/c1-3-4-5-23-7(21)6-20(2)14(22)8-9(15)11(17)13(19)12(18)10(8
InchiKey: XAPWDOHNXMABAC-UHFFFAOYSA-N
Formula: C14H14F5NO3
SMILES: CCCCOC(=O)CN(C)C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 339.26

Physical Properties

Property code	Value	Unit	Source
gf	-1094.85	kJ/mol	Joback Method
hf	-1423.51	kJ/mol	Joback Method
hfus	46.92	kJ/mol	Joback Method
hvap	66.20	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	2.797		Crippen Method
mcvol	212.200	ml/mol	McGowan Method
pc	1701.90	kPa	Joback Method
rinpol	1782.00		NIST Webbook
rinpol	1782.00		NIST Webbook
tb	710.25	K	Joback Method
tc	887.26	K	Joback Method
tf	494.07	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.39	J/mol×K	710.25	Joback Method
cpg	600.26	J/mol×K	739.75	Joback Method
cpg	611.48	J/mol×K	769.25	Joback Method
cpg	622.06	J/mol×K	798.75	Joback Method
cpg	632.01	J/mol×K	828.26	Joback Method
cpg	641.34	J/mol×K	857.76	Joback Method
cpg	650.05	J/mol×K	887.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321544&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