Sarcosine, n-pentafluorobenzoyl-, pentyl ester

Inchi: InChI=1S/C15H16F5NO3/c1-3-4-5-6-24-8(22)7-21(2)15(23)9-10(16)12(18)14(20)13(19)1
InchiKey: GJJHWKNRAVEFLG-UHFFFAOYSA-N
Formula: C15H16F5NO3
SMILES: CCCCCOC(=O)CN(C)C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 353.28

Physical Properties

Property code	Value	Unit	Source
gf	-1086.43	kJ/mol	Joback Method
hf	-1444.15	kJ/mol	Joback Method
hfus	49.51	kJ/mol	Joback Method
hvap	68.43	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.188		Crippen Method
mcvol	226.290	ml/mol	McGowan Method
pc	1574.70	kPa	Joback Method
rinpol	1872.00		NIST Webbook
rinpol	1872.00		NIST Webbook
tb	733.13	K	Joback Method
tc	910.76	K	Joback Method
tf	505.34	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.84	J/mol×K	733.13	Joback Method
cpg	654.24	J/mol×K	762.73	Joback Method
cpg	665.94	J/mol×K	792.34	Joback Method
cpg	676.97	J/mol×K	821.94	Joback Method
cpg	687.32	J/mol×K	851.55	Joback Method
cpg	697.00	J/mol×K	881.15	Joback Method
cpg	706.03	J/mol×K	910.76	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=U321545&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