Sarcosine, n-pentafluoropropionyl-, heptyl ester

Inchi: InChI=1S/C13H20F5NO3/c1-3-4-5-6-7-8-22-10(20)9-19(2)11(21)12(14,15)13(16,17)18/h

InchiKey: PJEMFNQVJAZNPJ-UHFFFAOYSA-N

Formula: C13H20F5NO3

SMILES: CCCCCCCOC(=O)CN(C)C(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 333.29

Physical Properties

Property code	Value	Unit	Source
gf	-1161.85	kJ/mol	Joback Method
hf	-1599.55	kJ/mol	Joback Method
hfus	37.40	kJ/mol	Joback Method
hvap	55.80	kJ/mol	Joback Method
log10ws	-3.45		Crippen Method
logp	3.156		Crippen Method
mcvol	221.870	ml/mol	McGowan Method
pc	1542.71	kPa	Joback Method
rinpol	1552.00		NIST Webbook
rinpol	1552.00		NIST Webbook
tb	629.33	K	Joback Method
tc	790.37	K	Joback Method
tf	398.62	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.87	J/mol×K	629.33	Joback Method
cpg	638.87	J/mol×K	656.17	Joback Method
cpg	652.11	J/mol×K	683.01	Joback Method
cpg	664.63	J/mol×K	709.85	Joback Method
cpg	676.46	J/mol×K	736.69	Joback Method
cpg	687.64	J/mol×K	763.53	Joback Method
cpg	698.20	J/mol×K	790.37	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=U320940&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