Sarcosine, n-pentafluoropropionyl-, propyl ester

Inchi: InChI=1S/C9H12F5NO3/c1-3-4-18-6(16)5-15(2)7(17)8(10,11)9(12,13)14/h3-5H2,1-2H3
InchiKey: QETYKYOJQVUYGB-UHFFFAOYSA-N
Formula: C9H12F5NO3
SMILES: CCCOC(=O)CN(C)C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 277.19

Physical Properties

Property code	Value	Unit	Source
gf	-1195.53	kJ/mol	Joback Method
hf	-1516.99	kJ/mol	Joback Method
hfus	27.04	kJ/mol	Joback Method
hvap	46.90	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.596		Crippen Method
mcvol	165.510	ml/mol	McGowan Method
pc	2139.38	kPa	Joback Method
rinpol	1173.00		NIST Webbook
rinpol	1173.00		NIST Webbook
tb	537.81	K	Joback Method
tc	699.50	K	Joback Method
tf	353.54	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	425.86	J/mol×K	537.81	Joback Method
cpg	437.78	J/mol×K	564.76	Joback Method
cpg	449.04	J/mol×K	591.71	Joback Method
cpg	459.65	J/mol×K	618.66	Joback Method
cpg	469.64	J/mol×K	645.61	Joback Method
cpg	479.05	J/mol×K	672.55	Joback Method
cpg	487.89	J/mol×K	699.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320936&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

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