Sarcosine, n-pentafluoropropionyl-, hexyl ester

Inchi: InChI=1S/C12H18F5NO3/c1-3-4-5-6-7-21-9(19)8-18(2)10(20)11(13,14)12(15,16)17/h3-8

InchiKey: HZESFLLANFNAGC-UHFFFAOYSA-N

Formula: C12H18F5NO3

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

Mol. weight [g/mol]: 319.27

Physical Properties

Property code	Value	Unit	Source
gf	-1170.27	kJ/mol	Joback Method
hf	-1578.91	kJ/mol	Joback Method
hfus	34.81	kJ/mol	Joback Method
hvap	53.57	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.766		Crippen Method
mcvol	207.780	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
rinpol	1466.00		NIST Webbook
rinpol	1466.00		NIST Webbook
tb	606.45	K	Joback Method
tc	767.21	K	Joback Method
tf	387.35	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.97	J/mol×K	606.45	Joback Method
cpg	586.50	J/mol×K	633.24	Joback Method
cpg	599.30	J/mol×K	660.04	Joback Method
cpg	611.40	J/mol×K	686.83	Joback Method
cpg	622.83	J/mol×K	713.62	Joback Method
cpg	633.61	J/mol×K	740.41	Joback Method
cpg	643.79	J/mol×K	767.21	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=U320939&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