Sarcosine, n-pentafluoropropionyl-, isohexyl ester

Inchi: InChI=1S/C12H18F5NO3/c1-8(2)5-4-6-21-9(19)7-18(3)10(20)11(13,14)12(15,16)17/h8H,

InchiKey: QSNDUJTVQYOINE-UHFFFAOYSA-N

Formula: C12H18F5NO3

SMILES: CC(C)CCCOC(=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	-1172.71	kJ/mol	Joback Method
hf	-1584.19	kJ/mol	Joback Method
hfus	31.29	kJ/mol	Joback Method
hvap	53.19	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.622		Crippen Method
mcvol	207.780	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	1414.00		NIST Webbook
rinpol	1414.00		NIST Webbook
tb	606.01	K	Joback Method
tc	769.01	K	Joback Method
tf	372.35	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.36	J/mol×K	606.01	Joback Method
cpg	587.13	J/mol×K	633.18	Joback Method
cpg	600.13	J/mol×K	660.34	Joback Method
cpg	612.41	J/mol×K	687.51	Joback Method
cpg	623.99	J/mol×K	714.67	Joback Method
cpg	634.92	J/mol×K	741.84	Joback Method
cpg	645.21	J/mol×K	769.01	Joback Method

Sources

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=U320938&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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