Sarcosine, n-heptafluorobutyryl-, isohexyl ester

Inchi: InChI=1S/C13H18F7NO3/c1-8(2)5-4-6-24-9(22)7-21(3)10(23)11(14,15)12(16,17)13(18,1

InchiKey: QYZDIFAFDRFMFB-UHFFFAOYSA-N

Formula: C13H18F7NO3

SMILES: CC(C)CCCOC(=O)CN(C)C(=O)C(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 369.28

Physical Properties

Property code	Value	Unit	Source
gf	-1551.07	kJ/mol	Joback Method
hf	-2005.80	kJ/mol	Joback Method
hfus	32.63	kJ/mol	Joback Method
hvap	52.48	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.257		Crippen Method
mcvol	225.410	ml/mol	McGowan Method
pc	1469.10	kPa	Joback Method
rinpol	1448.00		NIST Webbook
rinpol	1448.00		NIST Webbook
tb	624.20	K	Joback Method
tc	783.18	K	Joback Method
tf	387.22	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.21	J/mol×K	624.20	Joback Method
cpg	657.94	J/mol×K	650.70	Joback Method
cpg	670.86	J/mol×K	677.19	Joback Method
cpg	683.02	J/mol×K	703.69	Joback Method
cpg	694.46	J/mol×K	730.18	Joback Method
cpg	705.21	J/mol×K	756.68	Joback Method
cpg	715.32	J/mol×K	783.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321259&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