Sarcosine, n-heptafluorobutyryl-, pentyl ester

Inchi: InChI=1S/C12H16F7NO3/c1-3-4-5-6-23-8(21)7-20(2)9(22)10(13,14)11(15,16)12(17,18)1
InchiKey: OAZIBCRUEVFOKV-UHFFFAOYSA-N
Formula: C12H16F7NO3
SMILES: CCCCCOC(=O)CN(C)C(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 355.25

Physical Properties

Property code	Value	Unit	Source
gf	-1557.05	kJ/mol	Joback Method
hf	-1979.88	kJ/mol	Joback Method
hfus	33.56	kJ/mol	Joback Method
hvap	50.64	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.011		Crippen Method
mcvol	211.320	ml/mol	McGowan Method
pc	1573.45	kPa	Joback Method
rinpol	1395.00		NIST Webbook
rinpol	1395.00		NIST Webbook
tb	601.76	K	Joback Method
tc	758.26	K	Joback Method
tf	390.95	K	Joback Method
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	592.16	J/mol×K	601.76	Joback Method
cpg	605.26	J/mol×K	627.84	Joback Method
cpg	617.60	J/mol×K	653.93	Joback Method
cpg	629.21	J/mol×K	680.01	Joback Method
cpg	640.13	J/mol×K	706.09	Joback Method
cpg	650.39	J/mol×K	732.17	Joback Method
cpg	660.04	J/mol×K	758.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321258&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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