Sarcosine, n-pentafluoropropionyl-, isobutyl ester

Inchi: InChI=1S/C10H14F5NO3/c1-6(2)5-19-7(17)4-16(3)8(18)9(11,12)10(13,14)15/h6H,4-5H2

InchiKey: XDOPAQNMLRSEOO-UHFFFAOYSA-N

Formula: C10H14F5NO3

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

Mol. weight [g/mol]: 291.22

Physical Properties

Property code	Value	Unit	Source
gf	-1189.55	kJ/mol	Joback Method
hf	-1542.91	kJ/mol	Joback Method
hfus	26.11	kJ/mol	Joback Method
hvap	48.73	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.842		Crippen Method
mcvol	179.600	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
rinpol	1249.00		NIST Webbook
rinpol	1249.00		NIST Webbook
tb	560.25	K	Joback Method
tc	724.03	K	Joback Method
tf	349.81	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.71	J/mol×K	560.25	Joback Method
cpg	486.48	J/mol×K	587.55	Joback Method
cpg	498.52	J/mol×K	614.84	Joback Method
cpg	509.87	J/mol×K	642.14	Joback Method
cpg	520.57	J/mol×K	669.44	Joback Method
cpg	530.63	J/mol×K	696.74	Joback Method
cpg	540.08	J/mol×K	724.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U320937&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