Sarcosine, n-pentafluorobenzoyl-, octyl ester

Inchi: InChI=1S/C18H22F5NO3/c1-3-4-5-6-7-8-9-27-11(25)10-24(2)18(26)12-13(19)15(21)17(2
InchiKey: RNHUKAGPDAEJGV-UHFFFAOYSA-N
Formula: C18H22F5NO3
SMILES: CCCCCCCCOC(=O)CN(C)C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 395.36

Physical Properties

Property code	Value	Unit	Source
gf	-1061.17	kJ/mol	Joback Method
hf	-1506.07	kJ/mol	Joback Method
hfus	57.28	kJ/mol	Joback Method
hvap	75.11	kJ/mol	Joback Method
log10ws	-5.90		Crippen Method
logp	4.358		Crippen Method
mcvol	268.560	ml/mol	McGowan Method
pc	1268.25	kPa	Joback Method
rinpol	2164.00		NIST Webbook
rinpol	2164.00		NIST Webbook
tb	801.77	K	Joback Method
tc	984.86	K	Joback Method
tf	539.15	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	808.80	J/mol×K	801.77	Joback Method
cpg	822.67	J/mol×K	832.29	Joback Method
cpg	835.69	J/mol×K	862.80	Joback Method
cpg	847.87	J/mol×K	893.32	Joback Method
cpg	859.24	J/mol×K	923.83	Joback Method
cpg	869.81	J/mol×K	954.35	Joback Method
cpg	879.59	J/mol×K	984.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321549&Units=SI

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