Sarcosine, n-pentafluorobenzoyl-, heptadecyl ester

Inchi: InChI=1S/C27H40F5NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-36-20(34)19-33(

InchiKey: RIOWCAZMJMHIBB-UHFFFAOYSA-N

Formula: C27H40F5NO3

SMILES: CCCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 521.60

Physical Properties

Property code	Value	Unit	Source
gf	-985.39	kJ/mol	Joback Method
hf	-1691.83	kJ/mol	Joback Method
hfus	80.59	kJ/mol	Joback Method
hvap	95.14	kJ/mol	Joback Method
log10ws	-9.67		Crippen Method
logp	7.869		Crippen Method
mcvol	395.370	ml/mol	McGowan Method
pc	741.64	kPa	Joback Method
rinpol	3222.00		NIST Webbook
rinpol	3222.00		NIST Webbook
tb	1007.69	K	Joback Method
tc	1255.09	K	Joback Method
tf	640.58	K	Joback Method
vc	1.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1352.23	J/mol×K	1007.69	Joback Method
cpg	1371.22	J/mol×K	1048.92	Joback Method
cpg	1388.35	J/mol×K	1090.16	Joback Method
cpg	1403.71	J/mol×K	1131.39	Joback Method
cpg	1417.38	J/mol×K	1172.62	Joback Method
cpg	1429.46	J/mol×K	1213.86	Joback Method
cpg	1440.01	J/mol×K	1255.09	Joback Method

Sources

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=U321557&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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