Sarcosine, n-pentafluorobenzoyl-, hexadecyl ester

Inchi: InChI=1S/C26H38F5NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-35-19(33)18-32(2)2

InchiKey: IWJRXMYEYOMPBL-UHFFFAOYSA-N

Formula: C26H38F5NO3

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

Mol. weight [g/mol]: 507.58

Physical Properties

Property code	Value	Unit	Source
gf	-993.81	kJ/mol	Joback Method
hf	-1671.19	kJ/mol	Joback Method
hfus	78.00	kJ/mol	Joback Method
hvap	92.92	kJ/mol	Joback Method
log10ws	-9.25		Crippen Method
logp	7.479		Crippen Method
mcvol	381.280	ml/mol	McGowan Method
pc	782.00	kPa	Joback Method
rinpol	3046.00		NIST Webbook
tb	984.81	K	Joback Method
tc	1220.36	K	Joback Method
tf	629.31	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1289.61	J/mol×K	984.81	Joback Method
cpg	1307.89	J/mol×K	1024.07	Joback Method
cpg	1324.51	J/mol×K	1063.33	Joback Method
cpg	1339.51	J/mol×K	1102.58	Joback Method
cpg	1352.98	J/mol×K	1141.84	Joback Method
cpg	1364.98	J/mol×K	1181.10	Joback Method
cpg	1375.58	J/mol×K	1220.36	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=U321556&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