Sarcosine, n-pentafluoropropionyl-, hexadecyl ester

Inchi: InChI=1S/C22H38F5NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-31-19(29)18-28(2)2

InchiKey: GSGCQKPYPJZCRY-UHFFFAOYSA-N

Formula: C22H38F5NO3

SMILES: CCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 459.53

Physical Properties

Property code	Value	Unit	Source
gf	-1086.07	kJ/mol	Joback Method
hf	-1785.31	kJ/mol	Joback Method
hfus	60.71	kJ/mol	Joback Method
hvap	75.83	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.667		Crippen Method
mcvol	348.680	ml/mol	McGowan Method
pc	859.99	kPa	Joback Method
rinpol	2422.00		NIST Webbook
tb	835.25	K	Joback Method
tc	1023.47	K	Joback Method
tf	500.05	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1141.34	J/mol×K	835.25	Joback Method
cpg	1159.86	J/mol×K	866.62	Joback Method
cpg	1177.27	J/mol×K	897.99	Joback Method
cpg	1193.66	J/mol×K	929.36	Joback Method
cpg	1209.10	J/mol×K	960.73	Joback Method
cpg	1223.65	J/mol×K	992.10	Joback Method
cpg	1237.40	J/mol×K	1023.47	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=U320944&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