Sarcosine, n-pentafluorobenzoyl-, undecyl ester

Inchi: InChI=1S/C21H28F5NO3/c1-3-4-5-6-7-8-9-10-11-12-30-14(28)13-27(2)21(29)15-16(22)1

InchiKey: ZYFYDSRFTXTMBN-UHFFFAOYSA-N

Formula: C21H28F5NO3

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

Mol. weight [g/mol]: 437.44

Physical Properties

Property code	Value	Unit	Source
gf	-1035.91	kJ/mol	Joback Method
hf	-1567.99	kJ/mol	Joback Method
hfus	65.05	kJ/mol	Joback Method
hvap	81.79	kJ/mol	Joback Method
log10ws	-7.16		Crippen Method
logp	5.528		Crippen Method
mcvol	310.830	ml/mol	McGowan Method
pc	1043.27	kPa	Joback Method
rinpol	2462.00		NIST Webbook
tb	870.41	K	Joback Method
tc	1065.65	K	Joback Method
tf	572.96	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	984.04	J/mol×K	870.41	Joback Method
cpg	999.38	J/mol×K	902.95	Joback Method
cpg	1013.66	J/mol×K	935.49	Joback Method
cpg	1026.91	J/mol×K	968.03	Joback Method
cpg	1039.14	J/mol×K	1000.57	Joback Method
cpg	1050.39	J/mol×K	1033.11	Joback Method
cpg	1060.68	J/mol×K	1065.65	Joback Method

Sources

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=U321552&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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