Sarcosine, N-pentafluorobenzoyl-, nonyl ester

Inchi: InChI=1S/C19H24F5NO3/c1-3-4-5-6-7-8-9-10-28-12(26)11-25(2)19(27)13-14(20)16(22)1
InchiKey: WECVDIZBVLYKKH-UHFFFAOYSA-N
Formula: C19H24F5NO3
SMILES: CCCCCCCCCOC(=O)CN(C)C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 409.39

Physical Properties

Property code	Value	Unit	Source
hfus	59.87	kJ/mol	Joback Method
hvap	97.87	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.84		Cheméo Relay (1.0)
logp	4.748		Crippen Method
mcvol	282.650	ml/mol	McGowan Method
rinpol	2261.00		NIST Webbook
tb	614.43	K	Cheméo Relay (1.0)
tf	323.99	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	866.39	J/mol×K	824.65	Joback Method
cpg	880.74	J/mol×K	855.70	Joback Method
cpg	894.18	J/mol×K	886.76	Joback Method
cpg	906.72	J/mol×K	917.81	Joback Method
cpg	918.39	J/mol×K	948.86	Joback Method
cpg	929.20	J/mol×K	979.91	Joback Method
cpg	939.18	J/mol×K	1010.97	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321550&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point