

Sarcosine, n-pentafluorobenzoyl-, hexyl ester

Inchi:	InChI=1S/C16H18F5NO3/c1-3-4-5-6-7-25-9(23)8-22(2)16(24)10-11(17)13(19)15(21)14(2)
InchiKey:	CSRIUXJUHKNQST-UHFFFAOYSA-N
Formula:	C16H18F5NO3
SMILES:	CCCCCOC(=O)CN(C)C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	367.31

Physical Properties

Property code	Value	Unit	Source
gf	-1078.01	kJ/mol	Joback Method
hf	-1464.79	kJ/mol	Joback Method
hfus	52.10	kJ/mol	Joback Method
hvap	70.66	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	3.578		Crippen Method
mcvol	240.380	ml/mol	McGowan Method
pc	1461.25	kPa	Joback Method
rinsol	1966.00		NIST Webbook
tb	756.01	K	Joback Method
tc	934.82	K	Joback Method
tf	516.61	K	Joback Method
vc	0.962	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.44	J/mol×K	756.01	Joback Method
cpg	709.35	J/mol×K	785.81	Joback Method
cpg	721.51	J/mol×K	815.61	Joback Method
cpg	732.94	J/mol×K	845.41	Joback Method
cpg	743.66	J/mol×K	875.22	Joback Method
cpg	753.66	J/mol×K	905.02	Joback Method
cpg	762.97	J/mol×K	934.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321547&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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