Sarcosine, n-pentafluorobenzoyl-, heptyl ester

Inchi: InChI=1S/C17H20F5NO3/c1-3-4-5-6-7-8-26-10(24)9-23(2)17(25)11-12(18)14(20)16(22)1
InchiKey: JLWNPXMJESJVIE-UHFFFAOYSA-N
Formula: C17H20F5NO3
SMILES: CCCCCCCOC(=O)CN(C)C(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 381.34

Physical Properties

Property code	Value	Unit	Source
gf	-1069.59	kJ/mol	Joback Method
hf	-1485.43	kJ/mol	Joback Method
hfus	54.69	kJ/mol	Joback Method
hvap	72.88	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	3.968		Crippen Method
mcvol	254.470	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
rinpol	2067.00		NIST Webbook
rinpol	2067.00		NIST Webbook
tb	778.89	K	Joback Method
tc	959.50	K	Joback Method
tf	527.88	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.12	J/mol×K	778.89	Joback Method
cpg	765.51	J/mol×K	808.99	Joback Method
cpg	778.11	J/mol×K	839.09	Joback Method
cpg	789.93	J/mol×K	869.20	Joback Method
cpg	800.98	J/mol×K	899.30	Joback Method
cpg	811.28	J/mol×K	929.40	Joback Method
cpg	820.84	J/mol×K	959.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U321548&Units=SI
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

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

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