2-(Perfluorobenzamido)ethyl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C16H5F10NO3/c17-5-3(6(18)10(22)13(25)9(5)21)15(28)27-1-2-30-16(29)4-7(1

InchiKey: NZGGVEFBXKJOPQ-UHFFFAOYSA-N

Formula: C16H5F10NO3

SMILES: O=C(NCCOC(=O)c1c(F)c(F)c(F)c(F)c1F)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 449.20

Physical Properties

Property code	Value	Unit	Source
gf	-2009.19	kJ/mol	Joback Method
hf	-2280.22	kJ/mol	Joback Method
hfus	61.67	kJ/mol	Joback Method
hvap	76.55	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	3.664		Crippen Method
mcvol	225.470	ml/mol	McGowan Method
pc	1514.03	kPa	Joback Method
rinpol	2057.00		NIST Webbook
rinpol	2057.00		NIST Webbook
tb	841.67	K	Joback Method
tc	1032.44	K	Joback Method
tf	628.77	K	Joback Method
vc	0.961	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.98	J/mol×K	841.67	Joback Method
cpg	654.59	J/mol×K	873.47	Joback Method
cpg	662.47	J/mol×K	905.26	Joback Method
cpg	669.59	J/mol×K	937.06	Joback Method
cpg	675.96	J/mol×K	968.85	Joback Method
cpg	681.57	J/mol×K	1000.65	Joback Method
cpg	686.41	J/mol×K	1032.44	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373687&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