Pentafluorobenzoic acid, 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C12H3F13O2/c13-3-2(4(14)6(16)7(17)5(3)15)8(26)27-1-10(20,21)12(24,25)11(

InchiKey: UIAOMAFZCXDVJQ-UHFFFAOYSA-N

Formula: C12H3F13O2

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

Mol. weight [g/mol]: 426.13

Physical Properties

Property code	Value	Unit	Source
gf	-2645.95	kJ/mol	Joback Method
hf	-2937.59	kJ/mol	Joback Method
hfus	35.99	kJ/mol	Joback Method
hvap	42.15	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	4.710		Crippen Method
mcvol	186.630	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
rinpol	1192.00		NIST Webbook
rinpol	1192.00		NIST Webbook
tb	582.21	K	Joback Method
tc	730.88	K	Joback Method
tf	386.11	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.09	J/mol×K	582.21	Joback Method
cpg	518.57	J/mol×K	606.99	Joback Method
cpg	527.49	J/mol×K	631.77	Joback Method
cpg	535.87	J/mol×K	656.55	Joback Method
cpg	543.73	J/mol×K	681.32	Joback Method
cpg	551.10	J/mol×K	706.10	Joback Method
cpg	558.00	J/mol×K	730.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360620&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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