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

Inchi: InChI=1S/C12H6F10O2/c13-5-1-2-6(7(14)3-5)8(23)24-4-10(17,18)12(21,22)11(19,20)9(1

InchiKey: YXXJRJWUGWOKGP-UHFFFAOYSA-N

Formula: C12H6F10O2

SMILES: O=C(OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1ccc(F)cc1F

Mol. weight [g/mol]: 372.16

Physical Properties

Property code	Value	Unit	Source
gf	-2032.63	kJ/mol	Joback Method
hf	-2314.85	kJ/mol	Joback Method
hfus	27.92	kJ/mol	Joback Method
hvap	42.62	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.293		Crippen Method
mcvol	181.320	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	1288.00		NIST Webbook
tb	569.46	K	Joback Method
tc	730.78	K	Joback Method
tf	346.78	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.73	J/mol×K	569.46	Joback Method
cpg	496.99	J/mol×K	596.35	Joback Method
cpg	507.50	J/mol×K	623.23	Joback Method
cpg	517.31	J/mol×K	650.12	Joback Method
cpg	526.44	J/mol×K	677.01	Joback Method
cpg	534.94	J/mol×K	703.89	Joback Method
cpg	542.84	J/mol×K	730.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360552&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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