Fumaric acid, pentafluorobenzyl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C16H7F13O4/c17-8-5(9(18)11(20)12(21)10(8)19)3-32-6(30)1-2-7(31)33-4-14(2

InchiKey: VAQBXDABKIYEKT-OWOJBTEDSA-N

Formula: C16H7F13O4

SMILES: O=C(C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 510.20

Physical Properties

Property code	Value	Unit	Source
gf	-2765.97	kJ/mol	Joback Method
hf	-3147.73	kJ/mol	Joback Method
hfus	49.34	kJ/mol	Joback Method
hvap	60.17	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	4.696		Crippen Method
mcvol	246.130	ml/mol	McGowan Method
pc	1210.67	kPa	Joback Method
rinpol	1750.00		NIST Webbook
rinpol	1750.00		NIST Webbook
tb	754.18	K	Joback Method
tc	925.39	K	Joback Method
tf	498.27	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	727.71	J/mol×K	754.18	Joback Method
cpg	737.50	J/mol×K	782.72	Joback Method
cpg	746.60	J/mol×K	811.25	Joback Method
cpg	755.06	J/mol×K	839.79	Joback Method
cpg	762.90	J/mol×K	868.32	Joback Method
cpg	770.18	J/mol×K	896.86	Joback Method
cpg	776.93	J/mol×K	925.39	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405875&Units=SI

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