Fumaric acid, monoamide, N-(2-fluorophenyl)-, pentafluorobenzyl ester

Inchi: InChI=1S/C17H9F6NO3/c18-9-3-1-2-4-10(9)24-11(25)5-6-12(26)27-7-8-13(19)15(21)17(

InchiKey: TWIQGJNZRLXITI-AATRIKPKSA-N

Formula: C17H9F6NO3

SMILES: O=C(C=CC(=O)OCc1c(F)c(F)c(F)c(F)c1F)Nc1ccccc1F

Mol. weight [g/mol]: 389.25

Physical Properties

Property code	Value	Unit	Source
gf	-1102.79	kJ/mol	Joback Method
hf	-1353.32	kJ/mol	Joback Method
hfus	53.70	kJ/mol	Joback Method
hvap	79.35	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	3.759		Crippen Method
mcvol	228.180	ml/mol	McGowan Method
pc	1774.35	kPa	Joback Method
rinpol	2458.00		NIST Webbook
rinpol	2458.00		NIST Webbook
tb	851.71	K	Joback Method
tc	1056.11	K	Joback Method
tf	582.52	K	Joback Method
vc	0.924	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.72	J/mol×K	851.71	Joback Method
cpg	659.46	J/mol×K	885.78	Joback Method
cpg	668.38	J/mol×K	919.84	Joback Method
cpg	676.53	J/mol×K	953.91	Joback Method
cpg	683.92	J/mol×K	987.97	Joback Method
cpg	690.58	J/mol×K	1022.04	Joback Method
cpg	696.54	J/mol×K	1056.11	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=U357450&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