Fumaric acid, monoamide, N-methyl-N-phenyl-, pentafluorobenzyl ester

Inchi: InChI=1S/C18H12F5NO3/c1-24(10-5-3-2-4-6-10)12(25)7-8-13(26)27-9-11-14(19)16(21)1

InchiKey: ZWVQSLFQAZDRNB-BQYQJAHWSA-N

Formula: C18H12F5NO3

SMILES: CN(C(=O)C=CC(=O)OCc1c(F)c(F)c(F)c(F)c1F)c1ccccc1

Mol. weight [g/mol]: 385.28

Physical Properties

Property code	Value	Unit	Source
gf	-868.54	kJ/mol	Joback Method
hf	-1152.32	kJ/mol	Joback Method
hfus	51.52	kJ/mol	Joback Method
hvap	77.34	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	3.645		Crippen Method
mcvol	240.500	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
rinpol	2382.00		NIST Webbook
rinpol	2382.00		NIST Webbook
tb	832.61	K	Joback Method
tc	1036.84	K	Joback Method
tf	560.49	K	Joback Method
vc	0.946	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.02	J/mol×K	832.61	Joback Method
cpg	699.20	J/mol×K	866.65	Joback Method
cpg	709.51	J/mol×K	900.69	Joback Method
cpg	719.00	J/mol×K	934.73	Joback Method
cpg	727.71	J/mol×K	968.77	Joback Method
cpg	735.68	J/mol×K	1002.80	Joback Method
cpg	742.95	J/mol×K	1036.84	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=U357449&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