Fumaric acid, monoamide, N,N-dimethyl-, pentafluorobenzyl ester

Inchi: InChI=1S/C13H10F5NO3/c1-19(2)7(20)3-4-8(21)22-5-6-9(14)11(16)13(18)12(17)10(6)15

InchiKey: OTWMEKIYKLFHGX-ONEGZZNKSA-N

Formula: C13H10F5NO3

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

Mol. weight [g/mol]: 323.22

Physical Properties

Property code	Value	Unit	Source
gf	-1023.05	kJ/mol	Joback Method
hf	-1285.65	kJ/mol	Joback Method
hfus	44.53	kJ/mol	Joback Method
hvap	63.94	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	2.070		Crippen Method
mcvol	193.810	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	1981.00		NIST Webbook
rinpol	1981.00		NIST Webbook
tb	691.53	K	Joback Method
tc	873.53	K	Joback Method
tf	477.72	K	Joback Method
vc	0.773	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.06	J/mol×K	691.53	Joback Method
cpg	523.76	J/mol×K	721.86	Joback Method
cpg	533.85	J/mol×K	752.20	Joback Method
cpg	543.36	J/mol×K	782.53	Joback Method
cpg	552.30	J/mol×K	812.86	Joback Method
cpg	560.68	J/mol×K	843.19	Joback Method
cpg	568.51	J/mol×K	873.53	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=U357447&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