Fumaric acid, monoamide, N-(5-chloro-2-methoxyphenyl)-, pentafluorobenzyl ester

Inchi: InChI=1S/C18H11ClF5NO4/c1-28-11-3-2-8(19)6-10(11)25-12(26)4-5-13(27)29-7-9-14(20
InchiKey: VTZGYPOXVRDXHN-SNAWJCMRSA-N
Formula: C18H11ClF5NO4
SMILES: COc1ccc(Cl)cc1NC(=O)C=CC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 435.73

Physical Properties

Property code	Value	Unit	Source
gf	-1026.12	kJ/mol	Joback Method
hf	-1337.28	kJ/mol	Joback Method
hfus	58.21	kJ/mol	Joback Method
hvap	89.85	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	4.282		Crippen Method
mcvol	258.610	ml/mol	McGowan Method
pc	1607.71	kPa	Joback Method
rinpol	2974.00		NIST Webbook
rinpol	2974.00		NIST Webbook
tb	940.15	K	Joback Method
tc	1157.05	K	Joback Method
tf	657.87	K	Joback Method
vc	1.030	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.53	J/mol×K	940.15	Joback Method
cpg	749.36	J/mol×K	976.30	Joback Method
cpg	757.18	J/mol×K	1012.45	Joback Method
cpg	764.01	J/mol×K	1048.60	Joback Method
cpg	769.85	J/mol×K	1084.75	Joback Method
cpg	774.72	J/mol×K	1120.90	Joback Method
cpg	778.63	J/mol×K	1157.05	Joback Method

Sources

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=U357452&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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