Fumaric acid, pentafluorobenzyl 4-chloro-3-methylphenyl ester

Inchi: InChI=1S/C18H10ClF5O4/c1-8-6-9(2-3-11(8)19)28-13(26)5-4-12(25)27-7-10-14(20)16(22
InchiKey: KYJINWZVQHDSRM-SNAWJCMRSA-N
Formula: C18H10ClF5O4
SMILES: Cc1cc(OC(=O)C=CC(=O)OCc2c(F)c(F)c(F)c(F)c2F)ccc1Cl
Mol. weight [g/mol]: 420.71

Physical Properties

Property code	Value	Unit	Source
gf	-1115.51	kJ/mol	Joback Method
hf	-1390.75	kJ/mol	Joback Method
hfus	53.11	kJ/mol	Joback Method
hvap	83.42	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	4.549		Crippen Method
mcvol	248.630	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	2455.00		NIST Webbook
rinpol	2455.00		NIST Webbook
tb	889.98	K	Joback Method
tc	1101.71	K	Joback Method
tf	605.21	K	Joback Method
vc	0.995	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	691.06	J/mol×K	889.98	Joback Method
cpg	700.59	J/mol×K	925.27	Joback Method
cpg	709.19	J/mol×K	960.56	Joback Method
cpg	716.87	J/mol×K	995.84	Joback Method
cpg	723.63	J/mol×K	1031.13	Joback Method
cpg	729.49	J/mol×K	1066.42	Joback Method
cpg	734.46	J/mol×K	1101.71	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=U405883&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