Fumaric acid, pentafluorobenzyl 3-chlorophenyl ester

Inchi: InChI=1S/C17H8ClF5O4/c18-8-2-1-3-9(6-8)27-12(25)5-4-11(24)26-7-10-13(19)15(21)17(

InchiKey: YWGFYOJDDQSAEK-SNAWJCMRSA-N

Formula: C17H8ClF5O4

SMILES: O=C(C=CC(=O)Oc1cccc(Cl)c1)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 406.69

Physical Properties

Property code	Value	Unit	Source
gf	-1114.30	kJ/mol	Joback Method
hf	-1358.64	kJ/mol	Joback Method
hfus	50.91	kJ/mol	Joback Method
hvap	80.53	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	4.240		Crippen Method
mcvol	234.540	ml/mol	McGowan Method
pc	1741.91	kPa	Joback Method
rinpol	2299.00		NIST Webbook
rinpol	2299.00		NIST Webbook
tb	862.12	K	Joback Method
tc	1072.85	K	Joback Method
tf	581.42	K	Joback Method
vc	0.939	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.79	J/mol×K	862.12	Joback Method
cpg	647.05	J/mol×K	897.24	Joback Method
cpg	655.43	J/mol×K	932.36	Joback Method
cpg	662.96	J/mol×K	967.48	Joback Method
cpg	669.63	J/mol×K	1002.60	Joback Method
cpg	675.46	J/mol×K	1037.73	Joback Method
cpg	680.47	J/mol×K	1072.85	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405882&Units=SI
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

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