Fumaric acid, pentafluorobenzyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C17H7ClF6O4/c18-8-2-1-3-9(19)17(8)28-11(26)5-4-10(25)27-6-7-12(20)14(22)

InchiKey: XNJHDUTZRSLRHR-SNAWJCMRSA-N

Formula: C17H7ClF6O4

SMILES: O=C(C=CC(=O)Oc1c(F)cccc1Cl)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 424.68

Physical Properties

Property code	Value	Unit	Source
gf	-1318.74	kJ/mol	Joback Method
hf	-1566.22	kJ/mol	Joback Method
hfus	53.60	kJ/mol	Joback Method
hvap	80.38	kJ/mol	Joback Method
log10ws	-6.54		Crippen Method
logp	4.380		Crippen Method
mcvol	236.310	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	2250.00		NIST Webbook
rinpol	2250.00		NIST Webbook
tb	866.37	K	Joback Method
tc	1073.25	K	Joback Method
tf	594.53	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.48	J/mol×K	866.37	Joback Method
cpg	652.36	J/mol×K	900.85	Joback Method
cpg	660.39	J/mol×K	935.33	Joback Method
cpg	667.58	J/mol×K	969.81	Joback Method
cpg	673.94	J/mol×K	1004.29	Joback Method
cpg	679.47	J/mol×K	1038.77	Joback Method
cpg	684.19	J/mol×K	1073.25	Joback Method

Sources

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=U405881&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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