Fumaric acid, pentafluorobenzyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C17H7Cl2F5O4/c18-8-2-1-3-9(12(8)19)28-11(26)5-4-10(25)27-6-7-13(20)15(22
InchiKey: VTLHXUPVNYGRDE-SNAWJCMRSA-N
Formula: C17H7Cl2F5O4
SMILES: O=C(C=CC(=O)Oc1cccc(Cl)c1Cl)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 441.13

Physical Properties

Property code	Value	Unit	Source
gf	-1135.86	kJ/mol	Joback Method
hf	-1385.85	kJ/mol	Joback Method
hfus	54.71	kJ/mol	Joback Method
hvap	85.58	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	4.894		Crippen Method
mcvol	246.780	ml/mol	McGowan Method
pc	1668.70	kPa	Joback Method
rinpol	2493.00		NIST Webbook
tb	904.53	K	Joback Method
tc	1120.68	K	Joback Method
tf	623.86	K	Joback Method
vc	0.988	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.78	J/mol×K	904.53	Joback Method
cpg	662.92	J/mol×K	940.56	Joback Method
cpg	670.16	J/mol×K	976.58	Joback Method
cpg	676.51	J/mol×K	1012.61	Joback Method
cpg	681.98	J/mol×K	1048.63	Joback Method
cpg	686.58	J/mol×K	1084.66	Joback Method
cpg	690.32	J/mol×K	1120.68	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405884&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