Fumaric acid, pentafluorobenzyl 2,2-dichloroethyl ester

Inchi: InChI=1S/C13H7Cl2F5O4/c14-6(15)4-24-8(22)2-1-7(21)23-3-5-9(16)11(18)13(20)12(19)
InchiKey: BOJPTVVJOSWJQM-OWOJBTEDSA-N
Formula: C13H7Cl2F5O4
SMILES: O=C(C=CC(=O)OCC(Cl)Cl)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 393.09

Physical Properties

Property code	Value	Unit	Source
gf	-1265.13	kJ/mol	Joback Method
hf	-1522.16	kJ/mol	Joback Method
hfus	47.57	kJ/mol	Joback Method
hvap	72.69	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	3.328		Crippen Method
mcvol	214.180	ml/mol	McGowan Method
pc	1800.03	kPa	Joback Method
rinpol	1986.00		NIST Webbook
rinpol	1986.00		NIST Webbook
tb	775.93	K	Joback Method
tc	970.22	K	Joback Method
tf	512.32	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.79	J/mol×K	775.93	Joback Method
cpg	553.68	J/mol×K	808.31	Joback Method
cpg	561.92	J/mol×K	840.69	Joback Method
cpg	569.52	J/mol×K	873.07	Joback Method
cpg	576.48	J/mol×K	905.45	Joback Method
cpg	582.80	J/mol×K	937.83	Joback Method
cpg	588.50	J/mol×K	970.22	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405879&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