Fumaric acid, isobutyl pentachlorophenyl ester

Inchi: InChI=1S/C14H11Cl5O4/c1-6(2)5-22-7(20)3-4-8(21)23-14-12(18)10(16)9(15)11(17)13(14

InchiKey: RRORQPBYPGTCSN-ONEGZZNKSA-N

Formula: C14H11Cl5O4

SMILES: CC(C)COC(=O)C=CC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 420.50

Physical Properties

Property code	Value	Unit	Source
gf	-318.45	kJ/mol	Joback Method
hf	-609.47	kJ/mol	Joback Method
hfus	47.35	kJ/mol	Joback Method
hvap	92.15	kJ/mol	Joback Method
log10ws	-6.20		Crippen Method
logp	5.614		Crippen Method
mcvol	256.140	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	2649.00		NIST Webbook
rinpol	2649.00		NIST Webbook
tb	914.75	K	Joback Method
tc	1149.63	K	Joback Method
tf	610.40	K	Joback Method
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.52	J/mol×K	914.75	Joback Method
cpg	625.74	J/mol×K	953.90	Joback Method
cpg	633.02	J/mol×K	993.04	Joback Method
cpg	639.38	J/mol×K	1032.19	Joback Method
cpg	644.82	J/mol×K	1071.33	Joback Method
cpg	649.35	J/mol×K	1110.48	Joback Method
cpg	652.98	J/mol×K	1149.63	Joback Method
dvisc	0.0002670	Pa×s	610.40	Joback Method

dvisc	0.0001828	Pa×s	661.13	Joback Method
dvisc	0.0001321	Pa×s	711.85	Joback Method
dvisc	0.0000997	Pa×s	762.58	Joback Method
dvisc	0.0000779	Pa×s	813.30	Joback Method
dvisc	0.0000627	Pa×s	864.03	Joback Method
dvisc	0.0000517	Pa×s	914.75	Joback Method

Sources

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=U348180&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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