Fumaric acid, butyl pentachlorophenyl ester

Inchi: InChI=1S/C14H11Cl5O4/c1-2-3-6-22-7(20)4-5-8(21)23-14-12(18)10(16)9(15)11(17)13(14
InchiKey: FWAPVTJQGLXHOP-SNAWJCMRSA-N
Formula: C14H11Cl5O4
SMILES: CCCCOC(=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	-316.01	kJ/mol	Joback Method
hf	-604.19	kJ/mol	Joback Method
hfus	50.87	kJ/mol	Joback Method
hvap	92.54	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.758		Crippen Method
mcvol	256.140	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	2699.00		NIST Webbook
rinpol	2699.00		NIST Webbook
tb	915.19	K	Joback Method
tc	1147.20	K	Joback Method
tf	625.40	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.95	J/mol×K	915.19	Joback Method
cpg	625.11	J/mol×K	953.86	Joback Method
cpg	632.38	J/mol×K	992.53	Joback Method
cpg	638.76	J/mol×K	1031.19	Joback Method
cpg	644.26	J/mol×K	1069.86	Joback Method
cpg	648.88	J/mol×K	1108.53	Joback Method
cpg	652.63	J/mol×K	1147.20	Joback Method
dvisc	0.0002552	Pa×s	625.40	Joback Method

dvisc	0.0001815	Pa×s	673.70	Joback Method
dvisc	0.0001351	Pa×s	722.00	Joback Method
dvisc	0.0001043	Pa×s	770.30	Joback Method
dvisc	0.0000831	Pa×s	818.59	Joback Method
dvisc	0.0000678	Pa×s	866.89	Joback Method
dvisc	0.0000566	Pa×s	915.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348181&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
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