Fumaric acid, isobutyl 2,3,4,5-tetrachlorophenyl ester

Inchi: InChI=1S/C14H12Cl4O4/c1-7(2)6-21-10(19)3-4-11(20)22-9-5-8(15)12(16)14(18)13(9)17/

InchiKey: LSWQEYJKXOOGPU-ONEGZZNKSA-N

Formula: C14H12Cl4O4

SMILES: CC(C)COC(=O)C=CC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 386.06

Physical Properties

Property code	Value	Unit	Source
gf	-296.89	kJ/mol	Joback Method
hf	-582.26	kJ/mol	Joback Method
hfus	43.54	kJ/mol	Joback Method
hvap	87.10	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.961		Crippen Method
mcvol	243.900	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	2517.00		NIST Webbook
tb	872.34	K	Joback Method
tc	1103.40	K	Joback Method
tf	567.96	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.41	J/mol×K	872.34	Joback Method
cpg	610.79	J/mol×K	910.85	Joback Method
cpg	619.25	J/mol×K	949.36	Joback Method
cpg	626.80	J/mol×K	987.87	Joback Method
cpg	633.45	J/mol×K	1026.38	Joback Method
cpg	639.23	J/mol×K	1064.89	Joback Method
cpg	644.13	J/mol×K	1103.40	Joback Method
dvisc	0.0003504	Pa×s	567.96	Joback Method
dvisc	0.0002308	Pa×s	618.69	Joback Method

dvisc	0.0001619	Pa×s	669.42	Joback Method
dvisc	0.0001194	Pa×s	720.15	Joback Method
dvisc	0.0000917	Pa×s	770.88	Joback Method
dvisc	0.0000727	Pa×s	821.61	Joback Method
dvisc	0.0000593	Pa×s	872.34	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=U348241&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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