Fumaric acid, butyl 2,3,5,6-tetrachlorophenyl ester

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

InchiKey: ZGANIIKWTLMKME-SNAWJCMRSA-N

Formula: C14H12Cl4O4

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

Mol. weight [g/mol]: 386.06

Physical Properties

Property code	Value	Unit	Source
gf	-294.45	kJ/mol	Joback Method
hf	-576.98	kJ/mol	Joback Method
hfus	47.06	kJ/mol	Joback Method
hvap	87.49	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.105		Crippen Method
mcvol	243.900	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	2480.00		NIST Webbook
rinpol	2480.00		NIST Webbook
tb	872.78	K	Joback Method
tc	1100.74	K	Joback Method
tf	582.96	K	Joback Method
vc	0.935	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	600.80	J/mol×K	872.78	Joback Method
cpg	610.09	J/mol×K	910.77	Joback Method
cpg	618.50	J/mol×K	948.77	Joback Method
cpg	626.03	J/mol×K	986.76	Joback Method
cpg	632.71	J/mol×K	1024.75	Joback Method
cpg	638.54	J/mol×K	1062.74	Joback Method
cpg	643.53	J/mol×K	1100.74	Joback Method
dvisc	0.0003294	Pa×s	582.96	Joback Method

dvisc	0.0002264	Pa×s	631.26	Joback Method
dvisc	0.0001642	Pa×s	679.57	Joback Method
dvisc	0.0001242	Pa×s	727.87	Joback Method
dvisc	0.0000973	Pa×s	776.17	Joback Method
dvisc	0.0000785	Pa×s	824.48	Joback Method
dvisc	0.0000648	Pa×s	872.78	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=U348249&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