Fumaric acid, butyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C14H13Cl3O4/c1-2-3-6-20-13(18)4-5-14(19)21-12-8-10(16)9(15)7-11(12)17/h4
InchiKey: JCQGTZRZRUGTAR-SNAWJCMRSA-N
Formula: C14H13Cl3O4
SMILES: CCCCOC(=O)C=CC(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 351.61

Physical Properties

Property code	Value	Unit	Source
gf	-272.89	kJ/mol	Joback Method
hf	-549.77	kJ/mol	Joback Method
hfus	43.26	kJ/mol	Joback Method
hvap	82.44	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.452		Crippen Method
mcvol	231.660	ml/mol	McGowan Method
pc	1987.66	kPa	Joback Method
rinpol	2333.00		NIST Webbook
rinpol	2333.00		NIST Webbook
tb	830.37	K	Joback Method
tc	1054.44	K	Joback Method
tf	540.52	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.90	J/mol×K	830.37	Joback Method
cpg	626.32	J/mol×K	1017.10	Joback Method
cpg	619.33	J/mol×K	979.75	Joback Method
cpg	611.51	J/mol×K	942.41	Joback Method
cpg	602.84	J/mol×K	905.06	Joback Method
cpg	593.31	J/mol×K	867.72	Joback Method
cpg	632.50	J/mol×K	1054.44	Joback Method
dvisc	0.0000737	Pa×s	830.37	Joback Method

dvisc	0.0000903	Pa×s	782.06	Joback Method
dvisc	0.0001137	Pa×s	733.75	Joback Method
dvisc	0.0001479	Pa×s	685.45	Joback Method
dvisc	0.0002001	Pa×s	637.14	Joback Method
dvisc	0.0002846	Pa×s	588.83	Joback Method
dvisc	0.0004310	Pa×s	540.52	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=U348134&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