Fumaric acid, isobutyl 2,3,5-trichlorophenyl ester

Inchi: InChI=1S/C14H13Cl3O4/c1-8(2)7-20-12(18)3-4-13(19)21-11-6-9(15)5-10(16)14(11)17/h3

InchiKey: LEPGKNXBRAIHJE-ONEGZZNKSA-N

Formula: C14H13Cl3O4

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

Mol. weight [g/mol]: 351.61

Physical Properties

Property code	Value	Unit	Source
gf	-275.33	kJ/mol	Joback Method
hf	-555.05	kJ/mol	Joback Method
hfus	39.73	kJ/mol	Joback Method
hvap	82.06	kJ/mol	Joback Method
log10ws	-4.83		Crippen Method
logp	4.308		Crippen Method
mcvol	231.660	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	2268.00		NIST Webbook
rinpol	2268.00		NIST Webbook
tb	829.93	K	Joback Method
tc	1057.31	K	Joback Method
tf	525.52	K	Joback Method
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.51	J/mol×K	829.93	Joback Method
cpg	594.06	J/mol×K	867.83	Joback Method
cpg	603.69	J/mol×K	905.72	Joback Method
cpg	612.41	J/mol×K	943.62	Joback Method
cpg	620.25	J/mol×K	981.52	Joback Method
cpg	627.23	J/mol×K	1019.41	Joback Method
cpg	633.35	J/mol×K	1057.31	Joback Method
dvisc	0.0004680	Pa×s	525.52	Joback Method

dvisc	0.0002941	Pa×s	576.25	Joback Method
dvisc	0.0001993	Pa×s	626.99	Joback Method
dvisc	0.0001431	Pa×s	677.72	Joback Method
dvisc	0.0001076	Pa×s	728.46	Joback Method
dvisc	0.0000840	Pa×s	779.19	Joback Method
dvisc	0.0000676	Pa×s	829.93	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=U348141&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