Fumaric acid, 3,5-dichlorophenyl isobutyl ester

Inchi: InChI=1S/C14H14Cl2O4/c1-9(2)8-19-13(17)3-4-14(18)20-12-6-10(15)5-11(16)7-12/h3-7,

InchiKey: HLGHAOURNLIAIB-ONEGZZNKSA-N

Formula: C14H14Cl2O4

SMILES: CC(C)COC(=O)C=CC(=O)Oc1cc(Cl)cc(Cl)c1

Mol. weight [g/mol]: 317.17

Physical Properties

Property code	Value	Unit	Source
gf	-253.77	kJ/mol	Joback Method
hf	-527.84	kJ/mol	Joback Method
hfus	35.93	kJ/mol	Joback Method
hvap	77.01	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.654		Crippen Method
mcvol	219.420	ml/mol	McGowan Method
pc	2098.42	kPa	Joback Method
rinpol	2158.00		NIST Webbook
rinpol	2158.00		NIST Webbook
tb	787.52	K	Joback Method
tc	1011.27	K	Joback Method
tf	483.08	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.75	J/mol×K	787.52	Joback Method
cpg	575.48	J/mol×K	824.81	Joback Method
cpg	586.29	J/mol×K	862.10	Joback Method
cpg	596.19	J/mol×K	899.40	Joback Method
cpg	605.20	J/mol×K	936.69	Joback Method
cpg	613.35	J/mol×K	973.98	Joback Method
cpg	620.65	J/mol×K	1011.27	Joback Method
dvisc	0.0006394	Pa×s	483.08	Joback Method

dvisc	0.0003794	Pa×s	533.82	Joback Method
dvisc	0.0002464	Pa×s	584.56	Joback Method
dvisc	0.0001715	Pa×s	635.30	Joback Method
dvisc	0.0001259	Pa×s	686.04	Joback Method
dvisc	0.0000965	Pa×s	736.78	Joback Method
dvisc	0.0000765	Pa×s	787.52	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=U348233&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