Fumaric acid, butyl 3,5-dichlorophenyl ester

Inchi: InChI=1S/C14H14Cl2O4/c1-2-3-6-19-13(17)4-5-14(18)20-12-8-10(15)7-11(16)9-12/h4-5,
InchiKey: OWQDNEANEOIMEX-SNAWJCMRSA-N
Formula: C14H14Cl2O4
SMILES: CCCCOC(=O)C=CC(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 317.17

Physical Properties

Property code	Value	Unit	Source
gf	-251.33	kJ/mol	Joback Method
hf	-522.56	kJ/mol	Joback Method
hfus	39.45	kJ/mol	Joback Method
hvap	77.40	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.798		Crippen Method
mcvol	219.420	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	2201.00		NIST Webbook
rinpol	2201.00		NIST Webbook
tb	787.96	K	Joback Method
tc	1008.22	K	Joback Method
tf	498.08	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	563.14	J/mol×K	787.96	Joback Method
cpg	574.70	J/mol×K	824.67	Joback Method
cpg	585.37	J/mol×K	861.38	Joback Method
cpg	595.17	J/mol×K	898.09	Joback Method
cpg	604.12	J/mol×K	934.80	Joback Method
cpg	612.24	J/mol×K	971.51	Joback Method
cpg	619.56	J/mol×K	1008.22	Joback Method
dvisc	0.0005743	Pa×s	498.08	Joback Method

dvisc	0.0003610	Pa×s	546.39	Joback Method
dvisc	0.0002447	Pa×s	594.71	Joback Method
dvisc	0.0001759	Pa×s	643.02	Joback Method
dvisc	0.0001324	Pa×s	691.33	Joback Method
dvisc	0.0001034	Pa×s	739.65	Joback Method
dvisc	0.0000832	Pa×s	787.96	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=U348234&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