Fumaric acid, 3,5-dichlorophenyl ethyl ester

Inchi: InChI=1S/C12H10Cl2O4/c1-2-17-11(15)3-4-12(16)18-10-6-8(13)5-9(14)7-10/h3-7H,2H2,
InchiKey: NTLLZAXEGZZMPE-ONEGZZNKSA-N
Formula: C12H10Cl2O4
SMILES: CCOC(=O)C=CC(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 289.11

Physical Properties

Property code	Value	Unit	Source
gf	-268.17	kJ/mol	Joback Method
hf	-481.28	kJ/mol	Joback Method
hfus	34.27	kJ/mol	Joback Method
hvap	72.95	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.018		Crippen Method
mcvol	191.240	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
rinpol	1999.00		NIST Webbook
rinpol	1999.00		NIST Webbook
tb	742.20	K	Joback Method
tc	969.04	K	Joback Method
tf	475.54	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.46	J/mol×K	742.20	Joback Method
cpg	469.03	J/mol×K	780.01	Joback Method
cpg	478.79	J/mol×K	817.81	Joback Method
cpg	487.74	J/mol×K	855.62	Joback Method
cpg	495.91	J/mol×K	893.43	Joback Method
cpg	503.30	J/mol×K	931.24	Joback Method
cpg	509.93	J/mol×K	969.04	Joback Method
dvisc	0.0006727	Pa×s	475.54	Joback Method

dvisc	0.0004349	Pa×s	519.98	Joback Method
dvisc	0.0003012	Pa×s	564.43	Joback Method
dvisc	0.0002201	Pa×s	608.87	Joback Method
dvisc	0.0001678	Pa×s	653.31	Joback Method
dvisc	0.0001324	Pa×s	697.76	Joback Method
dvisc	0.0001075	Pa×s	742.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348231&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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