Fumaric acid, 3,5-dichlorophenyl propyl ester

Inchi: InChI=1S/C13H12Cl2O4/c1-2-5-18-12(16)3-4-13(17)19-11-7-9(14)6-10(15)8-11/h3-4,6-8
InchiKey: GQDYWAPQBXUEDV-ONEGZZNKSA-N
Formula: C13H12Cl2O4
SMILES: CCCOC(=O)C=CC(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 303.14

Physical Properties

Property code	Value	Unit	Source
gf	-259.75	kJ/mol	Joback Method
hf	-501.92	kJ/mol	Joback Method
hfus	36.86	kJ/mol	Joback Method
hvap	75.17	kJ/mol	Joback Method
log10ws	-3.96		Crippen Method
logp	3.408		Crippen Method
mcvol	205.330	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	2100.00		NIST Webbook
rinpol	2100.00		NIST Webbook
tb	765.08	K	Joback Method
tc	988.37	K	Joback Method
tf	486.81	K	Joback Method
vc	0.781	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	510.22	J/mol×K	765.08	Joback Method
cpg	521.32	J/mol×K	802.30	Joback Method
cpg	531.57	J/mol×K	839.51	Joback Method
cpg	540.98	J/mol×K	876.73	Joback Method
cpg	549.58	J/mol×K	913.94	Joback Method
cpg	557.37	J/mol×K	951.16	Joback Method
cpg	564.37	J/mol×K	988.37	Joback Method
dvisc	0.0006233	Pa×s	486.81	Joback Method

dvisc	0.0003973	Pa×s	533.19	Joback Method
dvisc	0.0002721	Pa×s	579.57	Joback Method
dvisc	0.0001972	Pa×s	625.95	Joback Method
dvisc	0.0001493	Pa×s	672.32	Joback Method
dvisc	0.0001172	Pa×s	718.70	Joback Method
dvisc	0.0000948	Pa×s	765.08	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=U348232&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

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