Fumaric acid, 3,5-dichlorophenyl heptyl ester

Inchi: InChI=1S/C17H20Cl2O4/c1-2-3-4-5-6-9-22-16(20)7-8-17(21)23-15-11-13(18)10-14(19)12
InchiKey: PKNSQHHAFHSLMA-BQYQJAHWSA-N
Formula: C17H20Cl2O4
SMILES: CCCCCCCOC(=O)C=CC(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 359.24

Physical Properties

Property code	Value	Unit	Source
gf	-226.07	kJ/mol	Joback Method
hf	-584.48	kJ/mol	Joback Method
hfus	47.22	kJ/mol	Joback Method
hvap	84.08	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.969		Crippen Method
mcvol	261.690	ml/mol	McGowan Method
pc	1627.22	kPa	Joback Method
rinpol	2535.00		NIST Webbook
tb	856.60	K	Joback Method
tc	1071.26	K	Joback Method
tf	531.89	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.12	J/mol×K	856.60	Joback Method
cpg	740.71	J/mol×K	892.38	Joback Method
cpg	752.31	J/mol×K	928.15	Joback Method
cpg	762.96	J/mol×K	963.93	Joback Method
cpg	772.69	J/mol×K	999.71	Joback Method
cpg	781.52	J/mol×K	1035.48	Joback Method
cpg	789.49	J/mol×K	1071.26	Joback Method
dvisc	0.0004362	Pa×s	531.89	Joback Method
dvisc	0.0002637	Pa×s	586.01	Joback Method

dvisc	0.0001736	Pa×s	640.13	Joback Method
dvisc	0.0001220	Pa×s	694.24	Joback Method
dvisc	0.0000902	Pa×s	748.36	Joback Method
dvisc	0.0000695	Pa×s	802.48	Joback Method
dvisc	0.0000553	Pa×s	856.60	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348238&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

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