Fumaric acid, 8-chlorooctyl ethyl ester

Inchi: InChI=1S/C14H23ClO4/c1-2-18-13(16)9-10-14(17)19-12-8-6-4-3-5-7-11-15/h9-10H,2-8,1
InchiKey: PZWWEXQGKBYUIG-MDZDMXLPSA-N
Formula: C14H23ClO4
SMILES: CCOC(=O)C=CC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 290.78

Physical Properties

Property code	Value	Unit	Source
gf	-332.55	kJ/mol	Joback Method
hf	-720.41	kJ/mol	Joback Method
hfus	41.99	kJ/mol	Joback Method
hvap	69.41	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	3.228		Crippen Method
mcvol	230.940	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	2090.00		NIST Webbook
tb	713.89	K	Joback Method
tc	899.58	K	Joback Method
tf	416.70	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.40	J/mol×K	713.89	Joback Method
cpg	643.72	J/mol×K	744.84	Joback Method
cpg	657.28	J/mol×K	775.79	Joback Method
cpg	670.10	J/mol×K	806.74	Joback Method
cpg	682.19	J/mol×K	837.68	Joback Method
cpg	693.58	J/mol×K	868.63	Joback Method
cpg	704.26	J/mol×K	899.58	Joback Method
dvisc	0.0011372	Pa×s	416.70	Joback Method
dvisc	0.0005993	Pa×s	466.23	Joback Method

dvisc	0.0003571	Pa×s	515.76	Joback Method
dvisc	0.0002330	Pa×s	565.29	Joback Method
dvisc	0.0001629	Pa×s	614.83	Joback Method
dvisc	0.0001201	Pa×s	664.36	Joback Method
dvisc	0.0000924	Pa×s	713.89	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348527&Units=SI

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