Fumaric acid, 2-chloropropyl hexyl ester

Inchi: InChI=1S/C13H21ClO4/c1-3-4-5-6-9-17-12(15)7-8-13(16)18-10-11(2)14/h7-8,11H,3-6,9-1
InchiKey: IXVHEHRRSGIADG-BQYQJAHWSA-N
Formula: C13H21ClO4
SMILES: CCCCCCOC(=O)C=CC(=O)OCC(C)Cl
Mol. weight [g/mol]: 276.76

Physical Properties

Property code	Value	Unit	Source
gf	-343.41	kJ/mol	Joback Method
hf	-705.05	kJ/mol	Joback Method
hfus	35.88	kJ/mol	Joback Method
hvap	66.80	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.837		Crippen Method
mcvol	216.850	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	1869.00		NIST Webbook
tb	690.57	K	Joback Method
tc	879.81	K	Joback Method
tf	390.43	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.14	J/mol×K	690.57	Joback Method
cpg	590.21	J/mol×K	722.11	Joback Method
cpg	603.52	J/mol×K	753.65	Joback Method
cpg	616.10	J/mol×K	785.19	Joback Method
cpg	627.95	J/mol×K	816.73	Joback Method
cpg	639.10	J/mol×K	848.27	Joback Method
cpg	649.56	J/mol×K	879.81	Joback Method
dvisc	0.0015002	Pa×s	390.43	Joback Method
dvisc	0.0007342	Pa×s	440.45	Joback Method

dvisc	0.0004157	Pa×s	490.48	Joback Method
dvisc	0.0002615	Pa×s	540.50	Joback Method
dvisc	0.0001779	Pa×s	590.52	Joback Method
dvisc	0.0001286	Pa×s	640.55	Joback Method
dvisc	0.0000974	Pa×s	690.57	Joback Method

Sources

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=U348564&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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