Fumaric acid, 2-chloropropyl heptyl ester

Inchi: InChI=1S/C14H23ClO4/c1-3-4-5-6-7-10-18-13(16)8-9-14(17)19-11-12(2)15/h8-9,12H,3-7
InchiKey: KFSJHJRXOISCGF-CMDGGOBGSA-N
Formula: C14H23ClO4
SMILES: CCCCCCCOC(=O)C=CC(=O)OCC(C)Cl
Mol. weight [g/mol]: 290.78

Physical Properties

Property code	Value	Unit	Source
gf	-334.99	kJ/mol	Joback Method
hf	-725.69	kJ/mol	Joback Method
hfus	38.47	kJ/mol	Joback Method
hvap	69.03	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.227		Crippen Method
mcvol	230.940	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	1973.00		NIST Webbook
rinpol	1973.00		NIST Webbook
tb	713.45	K	Joback Method
tc	901.62	K	Joback Method
tf	401.70	K	Joback Method
vc	0.890	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	629.92	J/mol×K	713.45	Joback Method
cpg	644.45	J/mol×K	744.81	Joback Method
cpg	658.19	J/mol×K	776.17	Joback Method
cpg	671.17	J/mol×K	807.53	Joback Method
cpg	683.39	J/mol×K	838.89	Joback Method
cpg	694.87	J/mol×K	870.25	Joback Method
cpg	705.63	J/mol×K	901.62	Joback Method
dvisc	0.0013688	Pa×s	401.70	Joback Method

dvisc	0.0006615	Pa×s	453.66	Joback Method
dvisc	0.0003712	Pa×s	505.62	Joback Method
dvisc	0.0002320	Pa×s	557.58	Joback Method
dvisc	0.0001571	Pa×s	609.53	Joback Method
dvisc	0.0001131	Pa×s	661.49	Joback Method
dvisc	0.0000854	Pa×s	713.45	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=U348565&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