Fumaric acid, 2-chloropropyl octyl ester

Inchi: InChI=1S/C15H25ClO4/c1-3-4-5-6-7-8-11-19-14(17)9-10-15(18)20-12-13(2)16/h9-10,13H
InchiKey: FJYBULSVGOZXRU-MDZDMXLPSA-N
Formula: C15H25ClO4
SMILES: CCCCCCCCOC(=O)C=CC(=O)OCC(C)Cl
Mol. weight [g/mol]: 304.81

Physical Properties

Property code	Value	Unit	Source
gf	-326.57	kJ/mol	Joback Method
hf	-746.33	kJ/mol	Joback Method
hfus	41.06	kJ/mol	Joback Method
hvap	71.25	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.617		Crippen Method
mcvol	245.030	ml/mol	McGowan Method
pc	1546.35	kPa	Joback Method
rinpol	2074.00		NIST Webbook
tb	736.33	K	Joback Method
tc	923.90	K	Joback Method
tf	412.97	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.90	J/mol×K	736.33	Joback Method
cpg	699.85	J/mol×K	767.59	Joback Method
cpg	713.98	J/mol×K	798.85	Joback Method
cpg	727.31	J/mol×K	830.11	Joback Method
cpg	739.86	J/mol×K	861.38	Joback Method
cpg	751.63	J/mol×K	892.64	Joback Method
cpg	762.66	J/mol×K	923.90	Joback Method
dvisc	0.0012420	Pa×s	412.97	Joback Method
dvisc	0.0005930	Pa×s	466.86	Joback Method

dvisc	0.0003299	Pa×s	520.76	Joback Method
dvisc	0.0002049	Pa×s	574.65	Joback Method
dvisc	0.0001381	Pa×s	628.54	Joback Method
dvisc	0.0000991	Pa×s	682.44	Joback Method
dvisc	0.0000746	Pa×s	736.33	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=U348566&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