Fumaric acid, 8-chlorooctyl propyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-324.13	kJ/mol	Joback Method
hf	-741.05	kJ/mol	Joback Method
hfus	44.58	kJ/mol	Joback Method
hvap	71.64	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.618		Crippen Method
mcvol	245.030	ml/mol	McGowan Method
pc	1536.66	kPa	Joback Method
rinpol	2191.00		NIST Webbook
rinpol	2191.00		NIST Webbook
tb	736.77	K	Joback Method
tc	922.13	K	Joback Method
tf	427.97	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.37	J/mol×K	736.77	Joback Method
cpg	699.13	J/mol×K	767.66	Joback Method
cpg	713.11	J/mol×K	798.56	Joback Method
cpg	726.30	J/mol×K	829.45	Joback Method
cpg	738.73	J/mol×K	860.35	Joback Method
cpg	750.42	J/mol×K	891.24	Joback Method
cpg	761.39	J/mol×K	922.13	Joback Method
dvisc	0.0010386	Pa×s	427.97	Joback Method

dvisc	0.0005401	Pa×s	479.44	Joback Method
dvisc	0.0003188	Pa×s	530.90	Joback Method
dvisc	0.0002066	Pa×s	582.37	Joback Method
dvisc	0.0001436	Pa×s	633.84	Joback Method
dvisc	0.0001055	Pa×s	685.30	Joback Method
dvisc	0.0000808	Pa×s	736.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348528&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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