Fumaric acid, 8-chlorooctyl nonyl ester

Inchi: InChI=1S/C21H37ClO4/c1-2-3-4-5-7-10-13-18-25-20(23)15-16-21(24)26-19-14-11-8-6-9-
InchiKey: WKCQJAPPHZEXMS-FOCLMDBBSA-N
Formula: C21H37ClO4
SMILES: CCCCCCCCCOC(=O)C=CC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 388.97

Physical Properties

Property code	Value	Unit	Source
gf	-273.61	kJ/mol	Joback Method
hf	-864.89	kJ/mol	Joback Method
hfus	60.12	kJ/mol	Joback Method
hvap	84.99	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.959		Crippen Method
mcvol	329.570	ml/mol	McGowan Method
pc	1022.69	kPa	Joback Method
rinpol	2804.00		NIST Webbook
rinpol	2804.00		NIST Webbook
tb	874.05	K	Joback Method
tc	1070.61	K	Joback Method
tf	495.59	K	Joback Method
vc	1.288	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1035.08	J/mol×K	874.05	Joback Method
cpg	1110.66	J/mol×K	1037.85	Joback Method
cpg	1097.59	J/mol×K	1005.09	Joback Method
cpg	1083.52	J/mol×K	972.33	Joback Method
cpg	1068.44	J/mol×K	939.57	Joback Method
cpg	1052.31	J/mol×K	906.81	Joback Method
cpg	1122.79	J/mol×K	1070.61	Joback Method
dvisc	0.0000342	Pa×s	874.05	Joback Method

dvisc	0.0000454	Pa×s	810.97	Joback Method
dvisc	0.0000631	Pa×s	747.90	Joback Method
dvisc	0.0000933	Pa×s	684.82	Joback Method
dvisc	0.0001493	Pa×s	621.74	Joback Method
dvisc	0.0002655	Pa×s	558.67	Joback Method
dvisc	0.0005469	Pa×s	495.59	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=U348536&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