Fumaric acid, 1-phenylprop-1-yl 8-chlorooctyl ester

Inchi: InChI=1S/C21H29ClO4/c1-2-19(18-12-8-7-9-13-18)26-21(24)15-14-20(23)25-17-11-6-4-3

InchiKey: XGBIGPAZRGKFGQ-CCEZHUSRSA-N

Formula: C21H29ClO4

SMILES: CCC(OC(=O)C=CC(=O)OCCCCCCCCCCl)c1ccccc1

Mol. weight [g/mol]: 380.91

Physical Properties

Property code	Value	Unit	Source
gf	-163.64	kJ/mol	Joback Method
hf	-633.64	kJ/mol	Joback Method
hfus	50.64	kJ/mol	Joback Method
hvap	86.88	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	5.360		Crippen Method
mcvol	305.810	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook
tb	900.29	K	Joback Method
tc	1111.07	K	Joback Method
tf	507.01	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	938.02	J/mol×K	900.29	Joback Method
cpg	1001.86	J/mol×K	1075.94	Joback Method
cpg	991.15	J/mol×K	1040.81	Joback Method
cpg	979.46	J/mol×K	1005.68	Joback Method
cpg	966.75	J/mol×K	970.55	Joback Method
cpg	952.95	J/mol×K	935.42	Joback Method
cpg	1011.64	J/mol×K	1111.07	Joback Method
dvisc	0.0000321	Pa×s	900.29	Joback Method

dvisc	0.0000425	Pa×s	834.74	Joback Method
dvisc	0.0000592	Pa×s	769.20	Joback Method
dvisc	0.0000877	Pa×s	703.65	Joback Method
dvisc	0.0001408	Pa×s	638.10	Joback Method
dvisc	0.0002520	Pa×s	572.56	Joback Method
dvisc	0.0005241	Pa×s	507.01	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=U405905&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