Fumaric acid, 2-isopropylphenyl 8-chlorooctyl ester

Inchi: InChI=1S/C21H29ClO4/c1-17(2)18-11-7-8-12-19(18)26-21(24)14-13-20(23)25-16-10-6-4

InchiKey: HQCKJPULXNIPCA-BUHFOSPRSA-N

Formula: C21H29ClO4

SMILES: CC(C)c1ccccc1OC(=O)C=CC(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 380.91

Physical Properties

Property code	Value	Unit	Source
gf	-173.27	kJ/mol	Joback Method
hf	-645.11	kJ/mol	Joback Method
hfus	50.25	kJ/mol	Joback Method
hvap	87.54	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.394		Crippen Method
mcvol	305.810	ml/mol	McGowan Method
pc	1272.78	kPa	Joback Method
rinpol	2761.00		NIST Webbook
rinpol	2761.00		NIST Webbook
tb	905.27	K	Joback Method
tc	1116.93	K	Joback Method
tf	519.53	K	Joback Method
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.13	J/mol×K	905.27	Joback Method
cpg	951.97	J/mol×K	940.55	Joback Method
cpg	965.68	J/mol×K	975.82	Joback Method
cpg	978.29	J/mol×K	1011.10	Joback Method
cpg	989.85	J/mol×K	1046.37	Joback Method
cpg	1000.40	J/mol×K	1081.65	Joback Method
cpg	1009.98	J/mol×K	1116.93	Joback Method
dvisc	0.0004472	Pa×s	519.53	Joback Method

dvisc	0.0002273	Pa×s	583.82	Joback Method
dvisc	0.0001322	Pa×s	648.11	Joback Method
dvisc	0.0000847	Pa×s	712.40	Joback Method
dvisc	0.0000585	Pa×s	776.69	Joback Method
dvisc	0.0000427	Pa×s	840.98	Joback Method
dvisc	0.0000326	Pa×s	905.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405871&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