Fumaric acid, 3-chlorophenyl 8-chlorooctyl ester

Inchi: InChI=1S/C18H22Cl2O4/c19-12-5-3-1-2-4-6-13-23-17(21)10-11-18(22)24-16-9-7-8-15(20

InchiKey: VGRWFVMJSRNTHU-ZHACJKMWSA-N

Formula: C18H22Cl2O4

SMILES: O=C(C=CC(=O)Oc1cccc(Cl)c1)OCCCCCCCCCl

Mol. weight [g/mol]: 373.27

Physical Properties

Property code	Value	Unit	Source
gf	-208.02	kJ/mol	Joback Method
hf	-593.65	kJ/mol	Joback Method
hfus	50.20	kJ/mol	Joback Method
hvap	85.64	kJ/mol	Joback Method
log10ws	-5.53		Crippen Method
logp	4.924		Crippen Method
mcvol	275.780	ml/mol	McGowan Method
pc	1525.88	kPa	Joback Method
rinpol	2797.00		NIST Webbook
rinpol	2797.00		NIST Webbook
tb	874.50	K	Joback Method
tc	1087.79	K	Joback Method
tf	530.64	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.17	J/mol×K	874.50	Joback Method
cpg	799.10	J/mol×K	910.05	Joback Method
cpg	811.02	J/mol×K	945.60	Joback Method
cpg	821.97	J/mol×K	981.14	Joback Method
cpg	831.99	J/mol×K	1016.69	Joback Method
cpg	841.12	J/mol×K	1052.24	Joback Method
cpg	849.39	J/mol×K	1087.79	Joback Method
dvisc	0.0004505	Pa×s	530.64	Joback Method

dvisc	0.0002576	Pa×s	587.95	Joback Method
dvisc	0.0001627	Pa×s	645.26	Joback Method
dvisc	0.0001107	Pa×s	702.57	Joback Method
dvisc	0.0000799	Pa×s	759.88	Joback Method
dvisc	0.0000603	Pa×s	817.19	Joback Method
dvisc	0.0000472	Pa×s	874.50	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=U405855&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