Fumaric acid, 2,4-dichlorophenyl 8-chlorooctyl ester

Inchi: InChI=1S/C18H21Cl3O4/c19-11-5-3-1-2-4-6-12-24-17(22)9-10-18(23)25-16-8-7-14(20)13

InchiKey: MDGVUJHZYAIXEG-MDZDMXLPSA-N

Formula: C18H21Cl3O4

SMILES: O=C(C=CC(=O)Oc1ccc(Cl)cc1Cl)OCCCCCCCCCl

Mol. weight [g/mol]: 407.72

Physical Properties

Property code	Value	Unit	Source
gf	-229.58	kJ/mol	Joback Method
hf	-620.86	kJ/mol	Joback Method
hfus	54.01	kJ/mol	Joback Method
hvap	90.69	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.578		Crippen Method
mcvol	288.020	ml/mol	McGowan Method
pc	1465.73	kPa	Joback Method
rinpol	2928.00		NIST Webbook
rinpol	2928.00		NIST Webbook
tb	916.91	K	Joback Method
tc	1135.61	K	Joback Method
tf	573.08	K	Joback Method
vc	1.111	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.30	J/mol×K	916.91	Joback Method
cpg	819.05	J/mol×K	953.36	Joback Method
cpg	829.80	J/mol×K	989.81	Joback Method
cpg	839.57	J/mol×K	1026.26	Joback Method
cpg	848.41	J/mol×K	1062.71	Joback Method
cpg	856.35	J/mol×K	1099.16	Joback Method
cpg	863.43	J/mol×K	1135.61	Joback Method
dvisc	0.0003248	Pa×s	573.08	Joback Method

dvisc	0.0001967	Pa×s	630.38	Joback Method
dvisc	0.0001295	Pa×s	687.69	Joback Method
dvisc	0.0000909	Pa×s	744.99	Joback Method
dvisc	0.0000671	Pa×s	802.30	Joback Method
dvisc	0.0000516	Pa×s	859.60	Joback Method
dvisc	0.0000410	Pa×s	916.91	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=U405703&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