Fumaric acid, 2-(2-methoxyethyl)hexyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C19H24Cl2O5/c1-3-4-6-14(11-12-24-2)13-25-17(22)9-10-18(23)26-16-8-5-7-15

InchiKey: FOUMKUZOUGTVRY-MDZDMXLPSA-N

Formula: C19H24Cl2O5

SMILES: CCCCC(CCOC)COC(=O)C=CC(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 403.30

Physical Properties

Property code	Value	Unit	Source
gf	-316.67	kJ/mol	Joback Method
hf	-763.26	kJ/mol	Joback Method
hfus	50.06	kJ/mol	Joback Method
hvap	90.55	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.841		Crippen Method
mcvol	295.740	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	2745.00		NIST Webbook
rinpol	2745.00		NIST Webbook
tb	924.34	K	Joback Method
tc	1141.47	K	Joback Method
tf	561.66	K	Joback Method
vc	1.129	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.07	J/mol×K	924.34	Joback Method
cpg	921.22	J/mol×K	1105.28	Joback Method
cpg	913.28	J/mol×K	1069.09	Joback Method
cpg	904.22	J/mol×K	1032.90	Joback Method
cpg	894.01	J/mol×K	996.72	Joback Method
cpg	882.63	J/mol×K	960.53	Joback Method
cpg	928.05	J/mol×K	1141.47	Joback Method
dvisc	0.0000282	Pa×s	924.34	Joback Method

dvisc	0.0000361	Pa×s	863.89	Joback Method
dvisc	0.0000478	Pa×s	803.45	Joback Method
dvisc	0.0000665	Pa×s	743.00	Joback Method
dvisc	0.0000979	Pa×s	682.55	Joback Method
dvisc	0.0001553	Pa×s	622.11	Joback Method
dvisc	0.0002723	Pa×s	561.66	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=U405893&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