Fumaric acid, 2-methylpentyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C16H18Cl2O4/c1-3-5-11(2)10-21-14(19)8-9-15(20)22-13-7-4-6-12(17)16(13)18

InchiKey: ZFIZWJDXTWUCJJ-CMDGGOBGSA-N

Formula: C16H18Cl2O4

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

Mol. weight [g/mol]: 345.22

Physical Properties

Property code	Value	Unit	Source
gf	-236.93	kJ/mol	Joback Method
hf	-569.12	kJ/mol	Joback Method
hfus	41.11	kJ/mol	Joback Method
hvap	81.46	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.434		Crippen Method
mcvol	247.600	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	2361.00		NIST Webbook
rinpol	2361.00		NIST Webbook
tb	833.28	K	Joback Method
tc	1052.04	K	Joback Method
tf	505.62	K	Joback Method
vc	0.944	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.75	J/mol×K	833.28	Joback Method
cpg	685.18	J/mol×K	869.74	Joback Method
cpg	696.62	J/mol×K	906.20	Joback Method
cpg	707.11	J/mol×K	942.66	Joback Method
cpg	716.66	J/mol×K	979.12	Joback Method
cpg	725.30	J/mol×K	1015.58	Joback Method
cpg	733.05	J/mol×K	1052.04	Joback Method
dvisc	0.0005311	Pa×s	505.62	Joback Method

dvisc	0.0003071	Pa×s	560.23	Joback Method
dvisc	0.0001957	Pa×s	614.84	Joback Method
dvisc	0.0001343	Pa×s	669.45	Joback Method
dvisc	0.0000975	Pa×s	724.06	Joback Method
dvisc	0.0000740	Pa×s	778.67	Joback Method
dvisc	0.0000583	Pa×s	833.28	Joback Method

Sources

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=U405652&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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