Fumaric acid, 2-chloro-5-methylphenyl isohexyl ester

Inchi: InChI=1S/C17H21ClO4/c1-12(2)5-4-10-21-16(19)8-9-17(20)22-15-11-13(3)6-7-14(15)18/

InchiKey: TYLIIEZFLRWKOL-CMDGGOBGSA-N

Formula: C17H21ClO4

SMILES: Cc1ccc(Cl)c(OC(=O)C=CC(=O)OCCCC(C)C)c1

Mol. weight [g/mol]: 324.80

Physical Properties

Property code	Value	Unit	Source
gf	-216.58	kJ/mol	Joback Method
hf	-574.02	kJ/mol	Joback Method
hfus	39.50	kJ/mol	Joback Method
hvap	79.30	kJ/mol	Joback Method
log10ws	-4.77		Crippen Method
logp	4.089		Crippen Method
mcvol	249.450	ml/mol	McGowan Method
pc	1687.95	kPa	Joback Method
rinpol	2303.00		NIST Webbook
rinpol	2303.00		NIST Webbook
tb	818.73	K	Joback Method
tc	1032.21	K	Joback Method
tf	486.97	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.73	J/mol×K	818.73	Joback Method
cpg	764.14	J/mol×K	996.63	Joback Method
cpg	754.19	J/mol×K	961.05	Joback Method
cpg	743.31	J/mol×K	925.47	Joback Method
cpg	731.45	J/mol×K	889.89	Joback Method
cpg	718.60	J/mol×K	854.31	Joback Method
cpg	773.17	J/mol×K	1032.21	Joback Method
dvisc	0.0000583	Pa×s	818.73	Joback Method

dvisc	0.0000745	Pa×s	763.44	Joback Method
dvisc	0.0000988	Pa×s	708.14	Joback Method
dvisc	0.0001375	Pa×s	652.85	Joback Method
dvisc	0.0002034	Pa×s	597.56	Joback Method
dvisc	0.0003260	Pa×s	542.26	Joback Method
dvisc	0.0005815	Pa×s	486.97	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=U348259&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