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

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

InchiKey: FAOAWVAOBJOJEV-MDZDMXLPSA-N

Formula: C17H21ClO4

SMILES: CCCCCCOC(=O)C=CC(=O)Oc1cc(C)ccc1Cl

Mol. weight [g/mol]: 324.80

Physical Properties

Property code	Value	Unit	Source
gf	-214.14	kJ/mol	Joback Method
hf	-568.74	kJ/mol	Joback Method
hfus	43.02	kJ/mol	Joback Method
hvap	79.69	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.234		Crippen Method
mcvol	249.450	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	2350.00		NIST Webbook
rinpol	2350.00		NIST Webbook
tb	819.17	K	Joback Method
tc	1029.92	K	Joback Method
tf	501.97	K	Joback Method
vc	0.957	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.17	J/mol×K	819.17	Joback Method
cpg	763.10	J/mol×K	994.79	Joback Method
cpg	753.18	J/mol×K	959.67	Joback Method
cpg	742.35	J/mol×K	924.54	Joback Method
cpg	730.59	J/mol×K	889.42	Joback Method
cpg	717.87	J/mol×K	854.29	Joback Method
cpg	772.14	J/mol×K	1029.92	Joback Method
dvisc	0.0000635	Pa×s	819.17	Joback Method

dvisc	0.0000799	Pa×s	766.30	Joback Method
dvisc	0.0001041	Pa×s	713.44	Joback Method
dvisc	0.0001413	Pa×s	660.57	Joback Method
dvisc	0.0002023	Pa×s	607.70	Joback Method
dvisc	0.0003102	Pa×s	554.84	Joback Method
dvisc	0.0005205	Pa×s	501.97	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=U348260&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