Fumaric acid, 3-methylbutyl 3-chlorophenyl ester

Inchi: InChI=1S/C15H17ClO4/c1-11(2)8-9-19-14(17)6-7-15(18)20-13-5-3-4-12(16)10-13/h3-7,1

InchiKey: PBMDALNQYYTTLJ-VOTSOKGWSA-N

Formula: C15H17ClO4

SMILES: CC(C)CCOC(=O)C=CC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 296.75

Physical Properties

Property code	Value	Unit	Source
gf	-223.79	kJ/mol	Joback Method
hf	-521.27	kJ/mol	Joback Method
hfus	34.71	kJ/mol	Joback Method
hvap	74.19	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.391		Crippen Method
mcvol	221.270	ml/mol	McGowan Method
pc	2016.32	kPa	Joback Method
rinpol	2073.00		NIST Webbook
rinpol	2073.00		NIST Webbook
tb	767.99	K	Joback Method
tc	985.06	K	Joback Method
tf	451.91	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.55	J/mol×K	767.99	Joback Method
cpg	608.89	J/mol×K	804.17	Joback Method
cpg	621.26	J/mol×K	840.35	Joback Method
cpg	632.68	J/mol×K	876.53	Joback Method
cpg	643.18	J/mol×K	912.71	Joback Method
cpg	652.79	J/mol×K	948.89	Joback Method
cpg	661.53	J/mol×K	985.06	Joback Method
dvisc	0.0008258	Pa×s	451.91	Joback Method

dvisc	0.0004501	Pa×s	504.59	Joback Method
dvisc	0.0002752	Pa×s	557.27	Joback Method
dvisc	0.0001831	Pa×s	609.95	Joback Method
dvisc	0.0001300	Pa×s	662.63	Joback Method
dvisc	0.0000971	Pa×s	715.31	Joback Method
dvisc	0.0000755	Pa×s	767.99	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=U405552&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