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

Inchi: InChI=1S/C15H17ClO4/c1-10(2)9-19-14(17)6-7-15(18)20-13-8-11(3)4-5-12(13)16/h4-8,1

InchiKey: QMXUCWZBIUTUSC-VOTSOKGWSA-N

Formula: C15H17ClO4

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

Mol. weight [g/mol]: 296.75

Physical Properties

Property code	Value	Unit	Source
gf	-233.42	kJ/mol	Joback Method
hf	-532.74	kJ/mol	Joback Method
hfus	34.32	kJ/mol	Joback Method
hvap	74.85	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.309		Crippen Method
mcvol	221.270	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	2087.00		NIST Webbook
tb	772.97	K	Joback Method
tc	990.82	K	Joback Method
tf	464.43	K	Joback Method
vc	0.839	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.33	J/mol×K	772.97	Joback Method
cpg	607.57	J/mol×K	809.28	Joback Method
cpg	619.86	J/mol×K	845.59	Joback Method
cpg	631.20	J/mol×K	881.89	Joback Method
cpg	641.63	J/mol×K	918.20	Joback Method
cpg	651.15	J/mol×K	954.51	Joback Method
cpg	659.80	J/mol×K	990.82	Joback Method
dvisc	0.0006946	Pa×s	464.43	Joback Method
dvisc	0.0003996	Pa×s	515.85	Joback Method

dvisc	0.0002541	Pa×s	567.28	Joback Method
dvisc	0.0001742	Pa×s	618.70	Joback Method
dvisc	0.0001266	Pa×s	670.12	Joback Method
dvisc	0.0000963	Pa×s	721.55	Joback Method
dvisc	0.0000759	Pa×s	772.97	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=U348256&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