Fumaric acid, 4-chlorophenyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C15H17ClO4/c1-10(2)11(3)19-14(17)8-9-15(18)20-13-6-4-12(16)5-7-13/h4-11H
InchiKey: MNNQONZPGLFYBU-CMDGGOBGSA-N
Formula: C15H17ClO4
SMILES: CC(C)C(C)OC(=O)C=CC(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 296.75

Physical Properties

Property code	Value	Unit	Source
gf	-226.23	kJ/mol	Joback Method
hf	-526.55	kJ/mol	Joback Method
hfus	31.18	kJ/mol	Joback Method
hvap	73.80	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.389		Crippen Method
mcvol	221.270	ml/mol	McGowan Method
pc	2030.89	kPa	Joback Method
rinpol	2057.00		NIST Webbook
rinpol	2057.00		NIST Webbook
tb	767.55	K	Joback Method
tc	988.14	K	Joback Method
tf	436.91	K	Joback Method
vc	0.833	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.13	J/mol×K	767.55	Joback Method
cpg	654.04	J/mol×K	951.37	Joback Method
cpg	644.38	J/mol×K	914.61	Joback Method
cpg	633.79	J/mol×K	877.84	Joback Method
cpg	622.24	J/mol×K	841.08	Joback Method
cpg	609.70	J/mol×K	804.31	Joback Method
cpg	662.79	J/mol×K	988.14	Joback Method
dvisc	0.0000695	Pa×s	767.55	Joback Method

dvisc	0.0000909	Pa×s	712.44	Joback Method
dvisc	0.0001244	Pa×s	657.34	Joback Method
dvisc	0.0001802	Pa×s	602.23	Joback Method
dvisc	0.0002814	Pa×s	547.12	Joback Method
dvisc	0.0004856	Pa×s	492.02	Joback Method
dvisc	0.0009615	Pa×s	436.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405841&Units=SI
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

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

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