Fumaric acid, 2-chlorophenyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C15H15ClO4/c1-11(2)9-10-19-14(17)7-8-15(18)20-13-6-4-3-5-12(13)16/h3-9H,

InchiKey: QQFACAHRIJYMLK-BQYQJAHWSA-N

Formula: C15H15ClO4

SMILES: CC(C)=CCOC(=O)C=CC(=O)Oc1ccccc1Cl

Mol. weight [g/mol]: 294.73

Physical Properties

Property code	Value	Unit	Source
gf	-149.68	kJ/mol	Joback Method
hf	-408.56	kJ/mol	Joback Method
hfus	37.12	kJ/mol	Joback Method
hvap	74.62	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	3.311		Crippen Method
mcvol	216.970	ml/mol	McGowan Method
pc	2108.07	kPa	Joback Method
rinpol	2126.00		NIST Webbook
rinpol	2126.00		NIST Webbook
tb	772.47	K	Joback Method
tc	996.23	K	Joback Method
tf	447.87	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.32	J/mol×K	772.47	Joback Method
cpg	582.05	J/mol×K	809.76	Joback Method
cpg	593.84	J/mol×K	847.06	Joback Method
cpg	604.76	J/mol×K	884.35	Joback Method
cpg	614.84	J/mol×K	921.64	Joback Method
cpg	624.13	J/mol×K	958.94	Joback Method
cpg	632.68	J/mol×K	996.23	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=U405721&Units=SI

Legend

cpg:	Ideal gas heat capacity
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