Fumaric acid, 1-phenylprop-1-yl 4-chloro-3-methylphenyl ester

Inchi: InChI=1S/C20H19ClO4/c1-3-18(15-7-5-4-6-8-15)25-20(23)12-11-19(22)24-16-9-10-17(21

InchiKey: PRTMDHCBQWMJIA-VAWYXSNFSA-N

Formula: C20H19ClO4

SMILES: CCC(OC(=O)C=CC(=O)Oc1ccc(Cl)c(C)c1)c1ccccc1

Mol. weight [g/mol]: 358.81

Physical Properties

Property code	Value	Unit	Source
gf	-78.91	kJ/mol	Joback Method
hf	-399.41	kJ/mol	Joback Method
hfus	41.31	kJ/mol	Joback Method
hvap	88.26	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	4.805		Crippen Method
mcvol	267.960	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinpol	2693.00		NIST Webbook
rinpol	2693.00		NIST Webbook
tb	914.05	K	Joback Method
tc	1150.88	K	Joback Method
tf	547.20	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.66	J/mol×K	914.05	Joback Method
cpg	788.15	J/mol×K	953.52	Joback Method
cpg	799.41	J/mol×K	992.99	Joback Method
cpg	809.50	J/mol×K	1032.47	Joback Method
cpg	818.48	J/mol×K	1071.94	Joback Method
cpg	826.40	J/mol×K	1111.41	Joback Method
cpg	833.33	J/mol×K	1150.88	Joback Method
dvisc	0.0003787	Pa×s	547.20	Joback Method

dvisc	0.0002151	Pa×s	608.34	Joback Method
dvisc	0.0001355	Pa×s	669.48	Joback Method
dvisc	0.0000922	Pa×s	730.62	Joback Method
dvisc	0.0000666	Pa×s	791.77	Joback Method
dvisc	0.0000504	Pa×s	852.91	Joback Method
dvisc	0.0000396	Pa×s	914.05	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=U405904&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