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

Inchi: InChI=1S/C14H15ClO4/c1-3-8-18-13(16)6-7-14(17)19-12-9-10(2)4-5-11(12)15/h4-7,9H,3

InchiKey: QOJOFIGGVFJBIJ-VOTSOKGWSA-N

Formula: C14H15ClO4

SMILES: CCCOC(=O)C=CC(=O)Oc1cc(C)ccc1Cl

Mol. weight [g/mol]: 282.72

Physical Properties

Property code	Value	Unit	Source
gf	-239.40	kJ/mol	Joback Method
hf	-506.82	kJ/mol	Joback Method
hfus	35.25	kJ/mol	Joback Method
hvap	73.01	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.063		Crippen Method
mcvol	207.180	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tb	750.53	K	Joback Method
tc	967.73	K	Joback Method
tf	468.16	K	Joback Method
vc	0.788	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.12	J/mol×K	750.53	Joback Method
cpg	552.75	J/mol×K	786.73	Joback Method
cpg	564.50	J/mol×K	822.93	Joback Method
cpg	575.37	J/mol×K	859.13	Joback Method
cpg	585.39	J/mol×K	895.33	Joback Method
cpg	594.58	J/mol×K	931.53	Joback Method
cpg	602.94	J/mol×K	967.73	Joback Method
dvisc	0.0006663	Pa×s	468.16	Joback Method

dvisc	0.0004136	Pa×s	515.22	Joback Method
dvisc	0.0002781	Pa×s	562.28	Joback Method
dvisc	0.0001988	Pa×s	609.35	Joback Method
dvisc	0.0001491	Pa×s	656.41	Joback Method
dvisc	0.0001163	Pa×s	703.47	Joback Method
dvisc	0.0000935	Pa×s	750.53	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=U348255&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