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

Inchi: InChI=1S/C13H13ClO4/c1-3-17-12(15)6-7-13(16)18-11-8-9(2)4-5-10(11)14/h4-8H,3H2,1

InchiKey: DHFVGVUEZZSWGO-VOTSOKGWSA-N

Formula: C13H13ClO4

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

Mol. weight [g/mol]: 268.69

Physical Properties

Property code	Value	Unit	Source
gf	-247.82	kJ/mol	Joback Method
hf	-486.18	kJ/mol	Joback Method
hfus	32.66	kJ/mol	Joback Method
hvap	70.79	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.673		Crippen Method
mcvol	193.090	ml/mol	McGowan Method
pc	2361.07	kPa	Joback Method
rinpol	1930.00		NIST Webbook
rinpol	1930.00		NIST Webbook
tb	727.65	K	Joback Method
tc	948.05	K	Joback Method
tf	456.89	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.67	J/mol×K	727.65	Joback Method
cpg	499.83	J/mol×K	764.38	Joback Method
cpg	511.12	J/mol×K	801.12	Joback Method
cpg	521.59	J/mol×K	837.85	Joback Method
cpg	531.23	J/mol×K	874.58	Joback Method
cpg	540.06	J/mol×K	911.32	Joback Method
cpg	548.09	J/mol×K	948.05	Joback Method
dvisc	0.0007152	Pa×s	456.89	Joback Method

dvisc	0.0004505	Pa×s	502.02	Joback Method
dvisc	0.0003062	Pa×s	547.14	Joback Method
dvisc	0.0002208	Pa×s	592.27	Joback Method
dvisc	0.0001667	Pa×s	637.40	Joback Method
dvisc	0.0001307	Pa×s	682.52	Joback Method
dvisc	0.0001055	Pa×s	727.65	Joback Method

Sources

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=U348254&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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