Fumaric acid, 2-methylpentyl 3-chlorophenyl ester

Inchi: InChI=1S/C16H19ClO4/c1-3-5-12(2)11-20-15(18)8-9-16(19)21-14-7-4-6-13(17)10-14/h4,

InchiKey: VDTRQVUSILCRFS-CMDGGOBGSA-N

Formula: C16H19ClO4

SMILES: CCCC(C)COC(=O)C=CC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 310.77

Physical Properties

Property code	Value	Unit	Source
gf	-215.37	kJ/mol	Joback Method
hf	-541.91	kJ/mol	Joback Method
hfus	37.30	kJ/mol	Joback Method
hvap	76.42	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.781		Crippen Method
mcvol	235.360	ml/mol	McGowan Method
pc	1853.11	kPa	Joback Method
rinpol	2168.00		NIST Webbook
rinpol	2168.00		NIST Webbook
tb	790.87	K	Joback Method
tc	1005.47	K	Joback Method
tf	463.18	K	Joback Method
vc	0.894	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.19	J/mol×K	790.87	Joback Method
cpg	708.83	J/mol×K	969.71	Joback Method
cpg	698.99	J/mol×K	933.94	Joback Method
cpg	688.23	J/mol×K	898.17	Joback Method
cpg	676.53	J/mol×K	862.40	Joback Method
cpg	663.86	J/mol×K	826.64	Joback Method
cpg	717.80	J/mol×K	1005.47	Joback Method
dvisc	0.0000661	Pa×s	790.87	Joback Method

dvisc	0.0000853	Pa×s	736.25	Joback Method
dvisc	0.0001147	Pa×s	681.64	Joback Method
dvisc	0.0001624	Pa×s	627.02	Joback Method
dvisc	0.0002458	Pa×s	572.41	Joback Method
dvisc	0.0004058	Pa×s	517.80	Joback Method
dvisc	0.0007540	Pa×s	463.18	Joback Method

Sources

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=U405650&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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