Fumaric acid, 4-chlorophenyl hept-2-yl ester

Inchi: InChI=1S/C17H21ClO4/c1-3-4-5-6-13(2)21-16(19)11-12-17(20)22-15-9-7-14(18)8-10-15/
InchiKey: FJYCRCIXAJCGDN-VAWYXSNFSA-N
Formula: C17H21ClO4
SMILES: CCCCCC(C)OC(=O)C=CC(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 324.80

Physical Properties

Property code	Value	Unit	Source
gf	-206.95	kJ/mol	Joback Method
hf	-562.55	kJ/mol	Joback Method
hfus	39.89	kJ/mol	Joback Method
hvap	78.64	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.314		Crippen Method
mcvol	249.450	ml/mol	McGowan Method
pc	1708.95	kPa	Joback Method
rinpol	2276.00		NIST Webbook
rinpol	2276.00		NIST Webbook
tb	813.75	K	Joback Method
tc	1026.45	K	Joback Method
tf	474.45	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.84	J/mol×K	813.75	Joback Method
cpg	765.67	J/mol×K	991.00	Joback Method
cpg	755.62	J/mol×K	955.55	Joback Method
cpg	744.65	J/mol×K	920.10	Joback Method
cpg	732.71	J/mol×K	884.65	Joback Method
cpg	719.79	J/mol×K	849.20	Joback Method
cpg	774.82	J/mol×K	1026.45	Joback Method
dvisc	0.0000577	Pa×s	813.75	Joback Method

dvisc	0.0000747	Pa×s	757.20	Joback Method
dvisc	0.0001009	Pa×s	700.65	Joback Method
dvisc	0.0001435	Pa×s	644.10	Joback Method
dvisc	0.0002186	Pa×s	587.55	Joback Method
dvisc	0.0003641	Pa×s	531.00	Joback Method
dvisc	0.0006850	Pa×s	474.45	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=U405842&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