Fumaric acid, 2,4-dimethylpent-3-yl hexyl ester

Inchi: InChI=1S/C17H30O4/c1-6-7-8-9-12-20-15(18)10-11-16(19)21-17(13(2)3)14(4)5/h10-11,1
InchiKey: WDPSXHOYSAAWSY-ZHACJKMWSA-N
Formula: C17H30O4
SMILES: CCCCCCOC(=O)C=CC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-302.68	kJ/mol	Joback Method
hf	-782.43	kJ/mol	Joback Method
hfus	34.99	kJ/mol	Joback Method
hvap	70.54	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.890		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1390.22	kPa	Joback Method
rinpol	1923.00		NIST Webbook
rinpol	1923.00		NIST Webbook
tb	743.78	K	Joback Method
tc	930.72	K	Joback Method
tf	375.59	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	768.78	J/mol×K	743.78	Joback Method
cpg	785.82	J/mol×K	774.94	Joback Method
cpg	801.94	J/mol×K	806.09	Joback Method
cpg	817.13	J/mol×K	837.25	Joback Method
cpg	831.44	J/mol×K	868.41	Joback Method
cpg	844.87	J/mol×K	899.56	Joback Method
cpg	857.44	J/mol×K	930.72	Joback Method
dvisc	0.0020291	Pa×s	375.59	Joback Method

dvisc	0.0007291	Pa×s	436.96	Joback Method
dvisc	0.0003371	Pa×s	498.32	Joback Method
dvisc	0.0001846	Pa×s	559.68	Joback Method
dvisc	0.0001138	Pa×s	621.05	Joback Method
dvisc	0.0000766	Pa×s	682.41	Joback Method
dvisc	0.0000550	Pa×s	743.78	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=U348547&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