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

Inchi: InChI=1S/C17H30O4/c1-12(2)8-7-11-20-15(18)9-10-16(19)21-17(13(3)4)14(5)6/h9-10,12

InchiKey: NWCXINUHLFDREU-MDZDMXLPSA-N

Formula: C17H30O4

SMILES: CC(C)CCCOC(=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	-305.12	kJ/mol	Joback Method
hf	-787.71	kJ/mol	Joback Method
hfus	31.47	kJ/mol	Joback Method
hvap	70.15	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.746		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1398.55	kPa	Joback Method
rinpol	1875.00		NIST Webbook
rinpol	1875.00		NIST Webbook
tb	743.34	K	Joback Method
tc	932.50	K	Joback Method
tf	360.59	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	769.28	J/mol×K	743.34	Joback Method
cpg	786.54	J/mol×K	774.87	Joback Method
cpg	802.83	J/mol×K	806.39	Joback Method
cpg	818.19	J/mol×K	837.92	Joback Method
cpg	832.62	J/mol×K	869.44	Joback Method
cpg	846.14	J/mol×K	900.97	Joback Method
cpg	858.79	J/mol×K	932.50	Joback Method
dvisc	0.0026689	Pa×s	360.59	Joback Method

dvisc	0.0008393	Pa×s	424.38	Joback Method
dvisc	0.0003571	Pa×s	488.17	Joback Method
dvisc	0.0001851	Pa×s	551.96	Joback Method
dvisc	0.0001100	Pa×s	615.76	Joback Method
dvisc	0.0000720	Pa×s	679.55	Joback Method
dvisc	0.0000507	Pa×s	743.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348546&Units=SI
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

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