Fumaric acid, 2,4,4-trimethylpentyl 3-methylbut-2-yl ester

Inchi: InChI=1S/C17H30O4/c1-12(2)14(4)21-16(19)9-8-15(18)20-11-13(3)10-17(5,6)7/h8-9,12-

InchiKey: ULINRDVYPHZRRN-CMDGGOBGSA-N

Formula: C17H30O4

SMILES: CC(COC(=O)C=CC(=O)OC(C)C(C)C)CC(C)(C)C

Mol. weight [g/mol]: 298.42

Physical Properties

Property code	Value	Unit	Source
gf	-299.84	kJ/mol	Joback Method
hf	-791.18	kJ/mol	Joback Method
hfus	27.58	kJ/mol	Joback Method
hvap	69.25	kJ/mol	Joback Method
log10ws	-3.90		Crippen Method
logp	3.746		Crippen Method
mcvol	260.970	ml/mol	McGowan Method
pc	1410.13	kPa	Joback Method
rinpol	1830.00		NIST Webbook
rinpol	1830.00		NIST Webbook
tb	740.55	K	Joback Method
tc	934.01	K	Joback Method
tf	378.01	K	Joback Method
vc	0.987	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.66	J/mol×K	740.55	Joback Method
cpg	847.81	J/mol×K	901.76	Joback Method
cpg	834.26	J/mol×K	869.52	Joback Method
cpg	819.80	J/mol×K	837.28	Joback Method
cpg	804.41	J/mol×K	805.04	Joback Method
cpg	788.04	J/mol×K	772.79	Joback Method
cpg	860.49	J/mol×K	934.01	Joback Method
dvisc	0.0000453	Pa×s	740.55	Joback Method

dvisc	0.0000648	Pa×s	680.13	Joback Method
dvisc	0.0000993	Pa×s	619.70	Joback Method
dvisc	0.0001669	Pa×s	559.28	Joback Method
dvisc	0.0003182	Pa×s	498.86	Joback Method
dvisc	0.0007244	Pa×s	438.43	Joback Method
dvisc	0.0021453	Pa×s	378.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405601&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

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