Fumaric acid, di(2,4,4-trimethylpentyl) ester

Inchi: InChI=1S/C20H36O4/c1-15(11-19(3,4)5)13-23-17(21)9-10-18(22)24-14-16(2)12-20(6,7)8
InchiKey: HFAKSYSFJUXFQY-MDZDMXLPSA-N
Formula: C20H36O4
SMILES: CC(COC(=O)C=CC(=O)OCC(C)CC(C)(C)C)CC(C)(C)C
Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-269.30	kJ/mol	Joback Method
hf	-856.57	kJ/mol	Joback Method
hfus	31.46	kJ/mol	Joback Method
hvap	75.02	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.774		Crippen Method
mcvol	303.240	ml/mol	McGowan Method
pc	1156.93	kPa	Joback Method
rinpol	2087.00		NIST Webbook
rinpol	2087.00		NIST Webbook
tb	806.40	K	Joback Method
tc	1002.80	K	Joback Method
tf	429.24	K	Joback Method
vc	1.149	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	947.01	J/mol×K	806.40	Joback Method
cpg	965.16	J/mol×K	839.13	Joback Method
cpg	982.21	J/mol×K	871.87	Joback Method
cpg	998.24	J/mol×K	904.60	Joback Method
cpg	1013.29	J/mol×K	937.33	Joback Method
cpg	1027.43	J/mol×K	970.06	Joback Method
cpg	1040.72	J/mol×K	1002.80	Joback Method
dvisc	0.0010923	Pa×s	429.24	Joback Method

dvisc	0.0003897	Pa×s	492.10	Joback Method
dvisc	0.0001756	Pa×s	554.96	Joback Method
dvisc	0.0000931	Pa×s	617.82	Joback Method
dvisc	0.0000555	Pa×s	680.68	Joback Method
dvisc	0.0000361	Pa×s	743.54	Joback Method
dvisc	0.0000251	Pa×s	806.40	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=U405617&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