Fumaric acid, di(2,4-dimethylpent-3-yl) ester

Inchi: InChI=1S/C18H32O4/c1-11(2)17(12(3)4)21-15(19)9-10-16(20)22-18(13(5)6)14(7)8/h9-14
InchiKey: GMAQGRKCHISKPO-MDZDMXLPSA-N
Formula: C18H32O4
SMILES: CC(C)C(OC(=O)C=CC(=O)OC(C(C)C)C(C)C)C(C)C
Mol. weight [g/mol]: 312.44

Physical Properties

Property code	Value	Unit	Source
gf	-301.58	kJ/mol	Joback Method
hf	-818.91	kJ/mol	Joback Method
hfus	27.01	kJ/mol	Joback Method
hvap	71.60	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.990		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1318.48	kPa	Joback Method
rinpol	1848.00		NIST Webbook
rinpol	1848.00		NIST Webbook
tb	765.34	K	Joback Method
tc	958.67	K	Joback Method
tf	341.86	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.19	J/mol×K	765.34	Joback Method
cpg	846.16	J/mol×K	797.56	Joback Method
cpg	863.06	J/mol×K	829.78	Joback Method
cpg	878.92	J/mol×K	862.00	Joback Method
cpg	893.76	J/mol×K	894.22	Joback Method
cpg	907.62	J/mol×K	926.45	Joback Method
cpg	920.50	J/mol×K	958.67	Joback Method
dvisc	0.0043884	Pa×s	341.86	Joback Method

dvisc	0.0010047	Pa×s	412.44	Joback Method
dvisc	0.0003539	Pa×s	483.02	Joback Method
dvisc	0.0001627	Pa×s	553.60	Joback Method
dvisc	0.0000891	Pa×s	624.18	Joback Method
dvisc	0.0000552	Pa×s	694.76	Joback Method
dvisc	0.0000373	Pa×s	765.34	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=U348562&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