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

Inchi: InChI=1S/C20H36O4/c1-6-7-8-9-10-11-12-15-23-18(21)13-14-19(22)24-20(16(2)3)17(4)5

InchiKey: OPDQFVGUOWUHDA-BUHFOSPRSA-N

Formula: C20H36O4

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

Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-277.42	kJ/mol	Joback Method
hf	-844.35	kJ/mol	Joback Method
hfus	42.76	kJ/mol	Joback Method
hvap	77.22	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	5.060		Crippen Method
mcvol	303.240	ml/mol	McGowan Method
pc	1133.67	kPa	Joback Method
rinpol	2217.00		NIST Webbook
rinpol	2217.00		NIST Webbook
tb	812.42	K	Joback Method
tc	1001.75	K	Joback Method
tf	409.40	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.33	J/mol×K	812.42	Joback Method
cpg	963.32	J/mol×K	843.98	Joback Method
cpg	980.24	J/mol×K	875.53	Joback Method
cpg	996.14	J/mol×K	907.09	Joback Method
cpg	1011.03	J/mol×K	938.64	Joback Method
cpg	1024.94	J/mol×K	970.20	Joback Method
cpg	1037.91	J/mol×K	1001.75	Joback Method
dvisc	0.0013918	Pa×s	409.40	Joback Method

dvisc	0.0004921	Pa×s	476.57	Joback Method
dvisc	0.0002250	Pa×s	543.74	Joback Method
dvisc	0.0001221	Pa×s	610.91	Joback Method
dvisc	0.0000749	Pa×s	678.08	Joback Method
dvisc	0.0000501	Pa×s	745.25	Joback Method
dvisc	0.0000358	Pa×s	812.42	Joback Method

Sources

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=U348550&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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