Fumaric acid, 4-methylpent-2-yl nonyl ester

Inchi: InChI=1S/C19H34O4/c1-5-6-7-8-9-10-11-14-22-18(20)12-13-19(21)23-17(4)15-16(2)3/h1
InchiKey: QUEAWVRHZOKWBN-OUKQBFOZSA-N
Formula: C19H34O4
SMILES: CCCCCCCCCOC(=O)C=CC(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 326.47

Physical Properties

Property code	Value	Unit	Source
gf	-283.40	kJ/mol	Joback Method
hf	-818.43	kJ/mol	Joback Method
hfus	43.70	kJ/mol	Joback Method
hvap	75.38	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.814		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1203.96	kPa	Joback Method
rinpol	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook
tb	789.98	K	Joback Method
tc	976.37	K	Joback Method
tf	413.13	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.08	J/mol×K	789.98	Joback Method
cpg	902.61	J/mol×K	821.05	Joback Method
cpg	919.15	J/mol×K	852.11	Joback Method
cpg	934.72	J/mol×K	883.18	Joback Method
cpg	949.36	J/mol×K	914.24	Joback Method
cpg	963.08	J/mol×K	945.31	Joback Method
cpg	975.91	J/mol×K	976.37	Joback Method
dvisc	0.0012655	Pa×s	413.13	Joback Method

dvisc	0.0005031	Pa×s	475.94	Joback Method
dvisc	0.0002480	Pa×s	538.75	Joback Method
dvisc	0.0001417	Pa×s	601.56	Joback Method
dvisc	0.0000900	Pa×s	664.36	Joback Method
dvisc	0.0000618	Pa×s	727.17	Joback Method
dvisc	0.0000451	Pa×s	789.98	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=U348323&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