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

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

Physical Properties

Property code	Value	Unit	Source
gf	-285.84	kJ/mol	Joback Method
hf	-823.71	kJ/mol	Joback Method
hfus	40.17	kJ/mol	Joback Method
hvap	74.99	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.670		Crippen Method
mcvol	289.150	ml/mol	McGowan Method
pc	1210.67	kPa	Joback Method
rinpol	2122.00		NIST Webbook
rinpol	2122.00		NIST Webbook
tb	789.54	K	Joback Method
tc	977.44	K	Joback Method
tf	398.13	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	885.58	J/mol×K	789.54	Joback Method
cpg	903.25	J/mol×K	820.86	Joback Method
cpg	919.91	J/mol×K	852.17	Joback Method
cpg	935.58	J/mol×K	883.49	Joback Method
cpg	950.29	J/mol×K	914.81	Joback Method
cpg	964.06	J/mol×K	946.12	Joback Method
cpg	976.92	J/mol×K	977.44	Joback Method
dvisc	0.0015838	Pa×s	398.13	Joback Method

dvisc	0.0005628	Pa×s	463.37	Joback Method
dvisc	0.0002582	Pa×s	528.60	Joback Method
dvisc	0.0001406	Pa×s	593.84	Joback Method
dvisc	0.0000863	Pa×s	659.07	Joback Method
dvisc	0.0000579	Pa×s	724.31	Joback Method
dvisc	0.0000415	Pa×s	789.54	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=U348549&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