Fumaric acid, 3-oxobut-2-yl undecyl ester

Inchi: InChI=1S/C19H32O5/c1-4-5-6-7-8-9-10-11-12-15-23-18(21)13-14-19(22)24-17(3)16(2)20
InchiKey: QQRTZCRDVYQBFJ-BUHFOSPRSA-N
Formula: C19H32O5
SMILES: CCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 340.45

Physical Properties

Property code	Value	Unit	Source
gf	-409.88	kJ/mol	Joback Method
hf	-925.73	kJ/mol	Joback Method
hfus	48.82	kJ/mol	Joback Method
hvap	82.52	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.137		Crippen Method
mcvol	290.720	ml/mol	McGowan Method
pc	1251.26	kPa	Joback Method
rinpol	2357.00		NIST Webbook
rinpol	2357.00		NIST Webbook
tb	844.29	K	Joback Method
tc	1038.44	K	Joback Method
tf	478.06	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.95	J/mol×K	844.29	Joback Method
cpg	921.91	J/mol×K	876.65	Joback Method
cpg	936.85	J/mol×K	909.01	Joback Method
cpg	950.78	J/mol×K	941.37	Joback Method
cpg	963.74	J/mol×K	973.72	Joback Method
cpg	975.76	J/mol×K	1006.08	Joback Method
cpg	986.85	J/mol×K	1038.44	Joback Method
dvisc	0.0007763	Pa×s	478.06	Joback Method

dvisc	0.0003729	Pa×s	539.10	Joback Method
dvisc	0.0002079	Pa×s	600.14	Joback Method
dvisc	0.0001291	Pa×s	661.17	Joback Method
dvisc	0.0000869	Pa×s	722.21	Joback Method
dvisc	0.0000622	Pa×s	783.25	Joback Method
dvisc	0.0000468	Pa×s	844.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348825&Units=SI
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

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