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

Inchi: InChI=1S/C27H48O5/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-31-26(29)21
InchiKey: IIMDZPHKOVFFPK-QURGRASLSA-N
Formula: C27H48O5
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 452.67

Physical Properties

Property code	Value	Unit	Source
gf	-342.52	kJ/mol	Joback Method
hf	-1090.85	kJ/mol	Joback Method
hfus	69.54	kJ/mol	Joback Method
hvap	100.32	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	7.258		Crippen Method
mcvol	403.440	ml/mol	McGowan Method
pc	773.75	kPa	Joback Method
rinpol	3161.00		NIST Webbook
rinpol	3161.00		NIST Webbook
tb	1027.33	K	Joback Method
tc	1270.28	K	Joback Method
tf	568.22	K	Joback Method
vc	1.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1400.55	J/mol×K	1027.33	Joback Method
cpg	1420.09	J/mol×K	1067.82	Joback Method
cpg	1437.83	J/mol×K	1108.31	Joback Method
cpg	1453.86	J/mol×K	1148.81	Joback Method
cpg	1468.27	J/mol×K	1189.30	Joback Method
cpg	1481.14	J/mol×K	1229.79	Joback Method
cpg	1492.57	J/mol×K	1270.28	Joback Method
dvisc	0.0002830	Pa×s	568.22	Joback Method

dvisc	0.0001267	Pa×s	644.74	Joback Method
dvisc	0.0000672	Pa×s	721.26	Joback Method
dvisc	0.0000403	Pa×s	797.77	Joback Method
dvisc	0.0000264	Pa×s	874.29	Joback Method
dvisc	0.0000185	Pa×s	950.81	Joback Method
dvisc	0.0000137	Pa×s	1027.33	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=U348833&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