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

Inchi: InChI=1S/C23H40O5/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19-27-22(25)17-18-23(26)28
InchiKey: RFWNPTLLHMDDFR-ISLYRVAYSA-N
Formula: C23H40O5
SMILES: CCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 396.56

Physical Properties

Property code	Value	Unit	Source
gf	-376.20	kJ/mol	Joback Method
hf	-1008.29	kJ/mol	Joback Method
hfus	59.18	kJ/mol	Joback Method
hvap	91.42	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	5.698		Crippen Method
mcvol	347.080	ml/mol	McGowan Method
pc	969.88	kPa	Joback Method
rinpol	2753.00		NIST Webbook
tb	935.81	K	Joback Method
tc	1145.98	K	Joback Method
tf	523.14	K	Joback Method
vc	1.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1148.88	J/mol×K	935.81	Joback Method
cpg	1223.70	J/mol×K	1110.95	Joback Method
cpg	1211.17	J/mol×K	1075.92	Joback Method
cpg	1197.47	J/mol×K	1040.89	Joback Method
cpg	1182.55	J/mol×K	1005.87	Joback Method
cpg	1166.37	J/mol×K	970.84	Joback Method
cpg	1235.09	J/mol×K	1145.98	Joback Method
dvisc	0.0000257	Pa×s	935.81	Joback Method
dvisc	0.0000345	Pa×s	867.03	Joback Method

dvisc	0.0000487	Pa×s	798.25	Joback Method
dvisc	0.0000733	Pa×s	729.48	Joback Method
dvisc	0.0001204	Pa×s	660.70	Joback Method
dvisc	0.0002218	Pa×s	591.92	Joback Method
dvisc	0.0004796	Pa×s	523.14	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=U348829&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