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

Inchi: InChI=1S/C21H36O5/c1-4-5-6-7-8-9-10-11-12-13-14-17-25-20(23)15-16-21(24)26-19(3)1
InchiKey: UHFHZYBUDDBCBR-FOCLMDBBSA-N
Formula: C21H36O5
SMILES: CCCCCCCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 368.51

Physical Properties

Property code	Value	Unit	Source
gf	-393.04	kJ/mol	Joback Method
hf	-967.01	kJ/mol	Joback Method
hfus	54.00	kJ/mol	Joback Method
hvap	86.97	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.918		Crippen Method
mcvol	318.900	ml/mol	McGowan Method
pc	1097.17	kPa	Joback Method
rinpol	2559.00		NIST Webbook
tb	890.05	K	Joback Method
tc	1090.41	K	Joback Method
tf	500.60	K	Joback Method
vc	1.240	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1026.10	J/mol×K	890.05	Joback Method
cpg	1098.37	J/mol×K	1057.02	Joback Method
cpg	1086.08	J/mol×K	1023.63	Joback Method
cpg	1072.74	J/mol×K	990.23	Joback Method
cpg	1058.32	J/mol×K	956.84	Joback Method
cpg	1042.79	J/mol×K	923.44	Joback Method
cpg	1109.64	J/mol×K	1090.41	Joback Method
dvisc	0.0000348	Pa×s	890.05	Joback Method
dvisc	0.0000465	Pa×s	825.14	Joback Method

dvisc	0.0000653	Pa×s	760.23	Joback Method
dvisc	0.0000978	Pa×s	695.33	Joback Method
dvisc	0.0001590	Pa×s	630.42	Joback Method
dvisc	0.0002892	Pa×s	565.51	Joback Method
dvisc	0.0006142	Pa×s	500.60	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=U348827&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