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

Inchi: InChI=1S/C16H26O5/c1-4-5-6-7-8-9-12-20-15(18)10-11-16(19)21-14(3)13(2)17/h10-11,1
InchiKey: HQFHXZPDBQRTDN-ZHACJKMWSA-N
Formula: C16H26O5
SMILES: CCCCCCCCOC(=O)C=CC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 298.37

Physical Properties

Property code	Value	Unit	Source
gf	-435.14	kJ/mol	Joback Method
hf	-863.81	kJ/mol	Joback Method
hfus	41.05	kJ/mol	Joback Method
hvap	75.84	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	2.967		Crippen Method
mcvol	248.450	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	2063.00		NIST Webbook
rinpol	2063.00		NIST Webbook
tb	775.65	K	Joback Method
tc	966.11	K	Joback Method
tf	444.25	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.77	J/mol×K	775.65	Joback Method
cpg	746.68	J/mol×K	807.39	Joback Method
cpg	760.71	J/mol×K	839.14	Joback Method
cpg	773.86	J/mol×K	870.88	Joback Method
cpg	786.17	J/mol×K	902.62	Joback Method
cpg	797.64	J/mol×K	934.37	Joback Method
cpg	808.30	J/mol×K	966.11	Joback Method
dvisc	0.0010714	Pa×s	444.25	Joback Method

dvisc	0.0005318	Pa×s	499.48	Joback Method
dvisc	0.0003035	Pa×s	554.72	Joback Method
dvisc	0.0001917	Pa×s	609.95	Joback Method
dvisc	0.0001307	Pa×s	665.18	Joback Method
dvisc	0.0000945	Pa×s	720.42	Joback Method
dvisc	0.0000716	Pa×s	775.65	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=U348822&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