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

Inchi: InChI=1S/C16H28O5/c1-4-5-6-7-8-9-12-20-15(18)10-11-16(19)21-14(3)13(2)17/h14H,4-1
InchiKey: SPAFUQKCFKORLB-UHFFFAOYSA-N
Formula: C16H28O5
SMILES: CCCCCCCCOC(=O)CCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 300.39

Physical Properties

Property code	Value	Unit	Source
gf	-515.36	kJ/mol	Joback Method
hf	-981.03	kJ/mol	Joback Method
hfus	40.85	kJ/mol	Joback Method
hvap	75.88	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.191		Crippen Method
mcvol	252.750	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
rinpol	2022.00		NIST Webbook
rinpol	2022.00		NIST Webbook
tb	771.49	K	Joback Method
tc	957.72	K	Joback Method
tf	449.33	K	Joback Method
vc	0.980	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	756.61	J/mol×K	771.49	Joback Method
cpg	772.06	J/mol×K	802.53	Joback Method
cpg	786.59	J/mol×K	833.57	Joback Method
cpg	800.23	J/mol×K	864.60	Joback Method
cpg	812.97	J/mol×K	895.64	Joback Method
cpg	824.83	J/mol×K	926.68	Joback Method
cpg	835.81	J/mol×K	957.72	Joback Method
dvisc	0.0011537	Pa×s	449.33	Joback Method

dvisc	0.0005879	Pa×s	503.02	Joback Method
dvisc	0.0003412	Pa×s	556.72	Joback Method
dvisc	0.0002179	Pa×s	610.41	Joback Method
dvisc	0.0001497	Pa×s	664.10	Joback Method
dvisc	0.0001087	Pa×s	717.80	Joback Method
dvisc	0.0000826	Pa×s	771.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349583&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