

Sebacic acid, di(3-oxobut-2-yl) ester

Inchi:	InChI=1S/C18H30O6/c1-13(19)15(3)23-17(21)11-9-7-5-6-8-10-12-18(22)24-16(4)14(2)20
InchiKey:	STLBYVLCPWJHCB-UHFFFAOYSA-N
Formula:	C18H30O6
SMILES:	CC(=O)C(C)OC(=O)CCCCCCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]:	342.43

Physical Properties

Property code	Value	Unit	Source
gf	-629.88	kJ/mol	Joback Method
hf	-1140.17	kJ/mol	Joback Method
hfus	44.10	kJ/mol	Joback Method
hvap	86.69	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	3.149		Crippen Method
mcvol	282.500	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
rinsol	2346.00		NIST Webbook
tb	870.68	K	Joback Method
tc	1070.14	K	Joback Method
tf	506.80	K	Joback Method
vc	1.091	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	891.54	J/molxK	870.68	Joback Method
cpg	906.17	J/molxK	903.92	Joback Method
cpg	919.66	J/molxK	937.17	Joback Method
cpg	932.04	J/molxK	970.41	Joback Method
cpg	943.30	J/molxK	1003.65	Joback Method
cpg	953.47	J/molxK	1036.90	Joback Method
cpg	962.56	J/molxK	1070.14	Joback Method
dvisc	0.0008243	Paxs	506.80	Joback Method
dvisc	0.0004102	Paxs	567.45	Joback Method

dvisc	0.0002335	Paxs	628.09	Joback Method
dvisc	0.0001468	Paxs	688.74	Joback Method
dvisc	0.0000995	Paxs	749.39	Joback Method
dvisc	0.0000715	Paxs	810.03	Joback Method
dvisc	0.0000538	Paxs	870.68	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=U355787&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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