Sebacic acid, butyl 3-oxobut-2-yl ester

Inchi: InChI=1S/C18H32O5/c1-4-5-14-22-17(20)12-10-8-6-7-9-11-13-18(21)23-16(3)15(2)19/h1
InchiKey: UYFJLCZXAVBUCI-UHFFFAOYSA-N
Formula: C18H32O5
SMILES: CCCCOC(=O)CCCCCCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 328.44

Physical Properties

Property code	Value	Unit	Source
gf	-498.52	kJ/mol	Joback Method
hf	-1022.31	kJ/mol	Joback Method
hfus	46.03	kJ/mol	Joback Method
hvap	80.33	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	3.971		Crippen Method
mcvol	280.930	ml/mol	McGowan Method
pc	1291.14	kPa	Joback Method
rinpol	2263.00		NIST Webbook
rinpol	2263.00		NIST Webbook
tb	817.25	K	Joback Method
tc	1006.29	K	Joback Method
tf	471.87	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.85	J/mol×K	817.25	Joback Method
cpg	889.00	J/mol×K	848.76	Joback Method
cpg	904.13	J/mol×K	880.26	Joback Method
cpg	918.25	J/mol×K	911.77	Joback Method
cpg	931.39	J/mol×K	943.28	Joback Method
cpg	943.54	J/mol×K	974.78	Joback Method
cpg	954.72	J/mol×K	1006.29	Joback Method
dvisc	0.0009340	Pa×s	471.87	Joback Method

dvisc	0.0004651	Pa×s	529.43	Joback Method
dvisc	0.0002655	Pa×s	587.00	Joback Method
dvisc	0.0001676	Pa×s	644.56	Joback Method
dvisc	0.0001140	Pa×s	702.12	Joback Method
dvisc	0.0000823	Pa×s	759.69	Joback Method
dvisc	0.0000621	Pa×s	817.25	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=U355775&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