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

Inchi: InChI=1S/C20H36O5/c1-4-5-6-13-16-24-19(22)14-11-9-7-8-10-12-15-20(23)25-18(3)17(2
InchiKey: CJEAVJFRXUHXFR-UHFFFAOYSA-N
Formula: C20H36O5
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]: 356.50

Physical Properties

Property code	Value	Unit	Source
gf	-481.68	kJ/mol	Joback Method
hf	-1063.59	kJ/mol	Joback Method
hfus	51.21	kJ/mol	Joback Method
hvap	84.78	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.751		Crippen Method
mcvol	309.110	ml/mol	McGowan Method
pc	1129.86	kPa	Joback Method
rinpol	2461.00		NIST Webbook
tb	863.01	K	Joback Method
tc	1057.77	K	Joback Method
tf	494.41	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.39	J/mol×K	863.01	Joback Method
cpg	1065.27	J/mol×K	1025.31	Joback Method
cpg	1052.93	J/mol×K	992.85	Joback Method
cpg	1039.49	J/mol×K	960.39	Joback Method
cpg	1024.93	J/mol×K	927.93	Joback Method
cpg	1009.24	J/mol×K	895.47	Joback Method
cpg	1076.52	J/mol×K	1057.77	Joback Method
dvisc	0.0000463	Pa×s	863.01	Joback Method
dvisc	0.0000616	Pa×s	801.58	Joback Method

dvisc	0.0000859	Pa×s	740.14	Joback Method
dvisc	0.0001273	Pa×s	678.71	Joback Method
dvisc	0.0002040	Pa×s	617.28	Joback Method
dvisc	0.0003626	Pa×s	555.84	Joback Method
dvisc	0.0007439	Pa×s	494.41	Joback Method

Sources

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=U355778&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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