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

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

Physical Properties

Property code	Value	Unit	Source
gf	-484.12	kJ/mol	Joback Method
hf	-1068.87	kJ/mol	Joback Method
hfus	47.68	kJ/mol	Joback Method
hvap	84.40	kJ/mol	Joback Method
log10ws	-5.07		Crippen Method
logp	4.607		Crippen Method
mcvol	309.110	ml/mol	McGowan Method
pc	1135.96	kPa	Joback Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook
tb	862.57	K	Joback Method
tc	1057.88	K	Joback Method
tf	479.41	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	992.87	J/mol×K	862.57	Joback Method
cpg	1009.76	J/mol×K	895.12	Joback Method
cpg	1025.47	J/mol×K	927.67	Joback Method
cpg	1040.03	J/mol×K	960.22	Joback Method
cpg	1053.45	J/mol×K	992.78	Joback Method
cpg	1065.76	J/mol×K	1025.33	Joback Method
cpg	1076.97	J/mol×K	1057.88	Joback Method
dvisc	0.0008629	Pa×s	479.41	Joback Method

dvisc	0.0003887	Pa×s	543.27	Joback Method
dvisc	0.0002071	Pa×s	607.13	Joback Method
dvisc	0.0001244	Pa×s	670.99	Joback Method
dvisc	0.0000816	Pa×s	734.85	Joback Method
dvisc	0.0000573	Pa×s	798.71	Joback Method
dvisc	0.0000424	Pa×s	862.57	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=U355777&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

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