

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

Inchi:	InChI=1S/C14H24O5/c1-4-5-6-7-10-18-13(16)8-9-14(17)19-12(3)11(2)15/h12H,4-10H2,1
InchiKey:	OPQHBBNKUMSRAL-UHFFFAOYSA-N
Formula:	C14H24O5
SMILES:	CCCCCOC(=O)CCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]:	272.34

Physical Properties

Property code	Value	Unit	Source
gf	-532.20	kJ/mol	Joback Method
hf	-939.75	kJ/mol	Joback Method
hfus	35.67	kJ/mol	Joback Method
hvap	71.43	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.411		Crippen Method
mcvol	224.570	ml/mol	McGowan Method
pc	1737.56	kPa	Joback Method
rinsol	1823.00		NIST Webbook
tb	725.73	K	Joback Method
tc	911.61	K	Joback Method
tf	426.79	K	Joback Method
vc	0.868	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.31	J/molxK	725.73	Joback Method
cpg	658.97	J/molxK	756.71	Joback Method
cpg	672.82	J/molxK	787.69	Joback Method
cpg	685.86	J/molxK	818.67	Joback Method
cpg	698.10	J/molxK	849.65	Joback Method
cpg	709.54	J/molxK	880.63	Joback Method
cpg	720.18	J/molxK	911.61	Joback Method
dvisc	0.0013982	Paxs	426.79	Joback Method
dvisc	0.0007307	Paxs	476.61	Joback Method

dvisc	0.0004318	Paxs	526.44	Joback Method
dvisc	0.0002795	Paxs	576.26	Joback Method
dvisc	0.0001938	Paxs	626.08	Joback Method
dvisc	0.0001419	Paxs	675.91	Joback Method
dvisc	0.0001084	Paxs	725.73	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U349581&Units=SI

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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