

Succinic acid, bis(2,2,4,4-tetra methyl-3-oxocyclobutyl) ester

Inchi: InChI=1S/C20H30O6/c1-17(2)12(18(3,4)14(17)23)13(22)25-10-9-11(21)26-16-19(5,6)15
InchiKey: GHHATPLUTKYQAZ-UHFFFAOYSA-N
Formula: C20H30O6
SMILES: CC1(C)C(=O)C(C)(C)C1OC(=O)CCOC(=O)C1C(C)(C)C(=O)C1(C)C
Mol. weight [g/mol]: 366.45

Physical Properties

Property code	Value	Unit	Source
gf	-551.00	kJ/mol	Joback Method
hf	-1108.25	kJ/mol	Joback Method
hfus	23.31	kJ/mol	Joback Method
hvap	81.25	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	2.718		Crippen Method
mcvol	288.960	ml/mol	McGowan Method
pc	1459.02	kPa	Joback Method
tb	949.52	K	Joback Method
tc	1184.89	K	Joback Method
tf	703.40	K	Joback Method
vc	1.103	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.86	J/molxK	949.52	Joback Method
cpg	1073.89	J/molxK	988.75	Joback Method
cpg	1107.96	J/molxK	1027.98	Joback Method
cpg	1144.46	J/molxK	1067.21	Joback Method
cpg	1183.80	J/molxK	1106.43	Joback Method
cpg	1226.37	J/molxK	1145.66	Joback Method
cpg	1272.55	J/molxK	1184.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6001741&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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