

Succinic acid, di(2,2-dimethylpent-3-yl) ester

Inchi: InChI=1S/C18H34O4/c1-9-13(17(3,4)5)21-15(19)11-12-16(20)22-14(10-2)18(6,7)8/h13-14
InchiKey: PAEKQZDNJDJDR-UHFFFAOYSA-N
Formula: C18H34O4
SMILES: CCC(OC(=O)CCC(=O)OC(CC)C(C)(C)C)C(C)(C)C
Mol. weight [g/mol]: 314.46

Physical Properties

Property code	Value	Unit	Source
gf	-366.36	kJ/mol	Joback Method
hf	-932.51	kJ/mol	Joback Method
hfus	26.08	kJ/mol	Joback Method
hvap	70.61	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	4.502		Crippen Method
mvol	279.360	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
rinpol	1817.00		NIST Webbook
rinpol	1817.00		NIST Webbook
tb	756.48	K	Joback Method
tc	948.35	K	Joback Method
tf	411.78	K	Joback Method
vc	1.058	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.62	J/molxK	756.48	Joback Method
cpg	934.27	J/molxK	916.37	Joback Method
cpg	920.13	J/molxK	884.39	Joback Method
cpg	905.05	J/molxK	852.42	Joback Method
cpg	888.96	J/molxK	820.44	Joback Method
cpg	871.84	J/molxK	788.46	Joback Method
cpg	947.48	J/molxK	948.35	Joback Method
dvisc	0.0000402	Paxs	756.48	Joback Method

dvisc	0.0000575	Paxs	699.03	Joback Method
dvisc	0.0000877	Paxs	641.58	Joback Method
dvisc	0.0001454	Paxs	584.13	Joback Method
dvisc	0.0002692	Paxs	526.68	Joback Method
dvisc	0.0005795	Paxs	469.23	Joback Method
dvisc	0.0015453	Paxs	411.78	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=U381738&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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