

Succinic acid, isobutyl pentyl ester

Other names:	Isobutyl pentyl succinate
Inchi:	InChI=1S/C13H24O4/c1-4-5-6-9-16-12(14)7-8-13(15)17-10-11(2)3/h11H,4-10H2,1-3H3
InchiKey:	UWFRUPKNEXYRBU-UHFFFAOYSA-N
Formula:	C13H24O4
SMILES:	CCCCCOC(=O)CCC(=O)OCC(C)C
Mol. weight [g/mol]:	244.33

Physical Properties

Property code	Value	Unit	Source
gf	-411.70	kJ/mol	Joback Method
hf	-806.53	kJ/mol	Joback Method
hfus	31.48	kJ/mol	Joback Method
hvap	62.46	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.699		Crippen Method
mvol	208.910	ml/mol	McGowan Method
pc	1786.37	kPa	Joback Method
ripol	1990.00		NIST Webbook
tb	648.98	K	Joback Method
tc	828.08	K	Joback Method
tf	365.59	K	Joback Method
vc	0.805	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.82	J/mol×K	648.98	Joback Method
cpg	584.20	J/mol×K	678.83	Joback Method
cpg	598.88	J/mol×K	708.68	Joback Method
cpg	612.86	J/mol×K	738.53	Joback Method
cpg	626.13	J/mol×K	768.38	Joback Method
cpg	638.71	J/mol×K	798.23	Joback Method
cpg	650.59	J/mol×K	828.08	Joback Method
dvisc	0.0019834	Paxs	365.59	Joback Method

dvisc	0.0009630	Paxs	412.82	Joback Method
dvisc	0.0005423	Paxs	460.05	Joback Method
dvisc	0.0003399	Paxs	507.29	Joback Method
dvisc	0.0002306	Paxs	554.52	Joback Method
dvisc	0.0001663	Paxs	601.75	Joback Method
dvisc	0.0001258	Paxs	648.98	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=U324971&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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