

Succinic acid, isobutyl pent-4-enyl ester

Inchi:	InChI=1S/C13H22O4/c1-4-5-6-9-16-12(14)7-8-13(15)17-10-11(2)3/h4,11H,1,5-10H2,2-3H1
InchiKey:	FMNPNJHLZSGMJ-UHFFFAOYSA-N
Formula:	C13H22O4
SMILES:	C=CCCCOC(=O)CCC(=O)OCC(C)C
Mol. weight [g/mol]:	242.31

Physical Properties

Property code	Value	Unit	Source
gf	-323.86	kJ/mol	Joback Method
hf	-681.10	kJ/mol	Joback Method
hfus	30.20	kJ/mol	Joback Method
hvap	61.79	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.475		Crippen Method
mvol	204.610	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rmpol	1599.00		NIST Webbook
tb	645.66	K	Joback Method
tc	827.30	K	Joback Method
tf	363.83	K	Joback Method
vc	0.786	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.28	J/molxK	645.66	Joback Method
cpg	613.53	J/molxK	797.03	Joback Method
cpg	601.47	J/molxK	766.76	Joback Method
cpg	588.71	J/molxK	736.48	Joback Method
cpg	575.27	J/molxK	706.21	Joback Method
cpg	561.13	J/molxK	675.93	Joback Method
cpg	624.91	J/molxK	827.30	Joback Method
dvisc	0.0001317	Paxs	645.66	Joback Method
dvisc	0.0001730	Paxs	598.69	Joback Method

dvisc	0.0002381	Paxs	551.72	Joback Method
dvisc	0.0003476	Paxs	504.75	Joback Method
dvisc	0.0005485	Paxs	457.77	Joback Method
dvisc	0.0009606	Paxs	410.80	Joback Method
dvisc	0.0019445	Paxs	363.83	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=U353369&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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