

Succinic acid, di(but-3-en-1-yl) ester

Inchi:	InChI=1S/C12H18O4/c1-3-5-9-15-11(13)7-8-12(14)16-10-6-4-2/h3-4H,1-2,5-10H2
InchiKey:	NJSWADUSSGQREI-UHFFFAOYSA-N
Formula:	C12H18O4
SMILES:	C=CCCOC(=O)CCC(=O)OCCC=C
Mol. weight [g/mol]:	226.27

Physical Properties

Property code	Value	Unit	Source
gf	-242.00	kJ/mol	Joback Method
hf	-529.75	kJ/mol	Joback Method
hfus	29.85	kJ/mol	Joback Method
hvap	59.28	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.005		Crippen Method
mcvol	186.220	ml/mol	McGowan Method
pc	2077.43	kPa	Joback Method
rinsol	1515.00		NIST Webbook
tb	619.90	K	Joback Method
tc	802.73	K	Joback Method
tf	365.80	K	Joback Method
vc	0.718	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.49	J/molxK	619.90	Joback Method
cpg	485.91	J/molxK	650.37	Joback Method
cpg	498.71	J/molxK	680.84	Joback Method
cpg	510.88	J/molxK	711.31	Joback Method
cpg	522.43	J/molxK	741.78	Joback Method
cpg	533.37	J/molxK	772.26	Joback Method
cpg	543.71	J/molxK	802.73	Joback Method
dvisc	0.0016394	Paxs	365.80	Joback Method
dvisc	0.0009174	Paxs	408.15	Joback Method

dvisc	0.0005726	Paxs	450.50	Joback Method
dvisc	0.0003875	Paxs	492.85	Joback Method
dvisc	0.0002790	Paxs	535.20	Joback Method
dvisc	0.0002108	Paxs	577.55	Joback Method
dvisc	0.0001655	Paxs	619.90	Joback Method

Sources

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=U391206&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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