

Succinic acid, ethyl trans-hex-3-enyl ester

Inchi:	InChI=1S/C12H20O4/c1-3-5-6-7-10-16-12(14)9-8-11(13)15-4-2/h5-6H,3-4,7-10H2,1-2H3
InchiKey:	WKZZFRSJSZINKQ-AATRIKPKSA-N
Formula:	C12H20O4
SMILES:	CCC=CCCOC(=O)CCC(=O)OCC
Mol. weight [g/mol]:	228.28

Physical Properties

Property code	Value	Unit	Source
gf	-337.46	kJ/mol	Joback Method
hf	-663.39	kJ/mol	Joback Method
hfus	32.61	kJ/mol	Joback Method
hvap	60.58	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.229		Crippen Method
mcvol	190.520	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinsol	1550.00		NIST Webbook
tb	630.70	K	Joback Method
tc	814.25	K	Joback Method
tf	364.24	K	Joback Method
vc	0.736	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.03	J/molxK	630.70	Joback Method
cpg	509.10	J/molxK	661.29	Joback Method
cpg	522.51	J/molxK	691.88	Joback Method
cpg	535.27	J/molxK	722.48	Joback Method
cpg	547.40	J/molxK	753.07	Joback Method
cpg	558.89	J/molxK	783.66	Joback Method
cpg	569.75	J/molxK	814.25	Joback Method
dvisc	0.0015837	Paxs	364.24	Joback Method
dvisc	0.0008330	Paxs	408.65	Joback Method

dvisc	0.0004970	Paxs	453.06	Joback Method
dvisc	0.0003252	Paxs	497.47	Joback Method
dvisc	0.0002281	Paxs	541.88	Joback Method
dvisc	0.0001688	Paxs	586.29	Joback Method
dvisc	0.0001303	Paxs	630.70	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=U353424&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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