

Succinic acid, 2-ethylhexyl hex-5-en-1-yl ester

Inchi:	InChI=1S/C18H32O4/c1-4-7-9-10-14-21-17(19)12-13-18(20)22-15-16(6-3)11-8-5-2/h4,16
InchiKey:	ZEDDXIPTSZFJQL-UHFFFAOYSA-N
Formula:	C18H32O4
SMILES:	C=CCCCCOC(=O)CCC(=O)OCC(CC)CCCC
Mol. weight [g/mol]:	312.44

Physical Properties

Property code	Value	Unit	Source
gf	-281.76	kJ/mol	Joback Method
hf	-784.30	kJ/mol	Joback Method
hfus	43.15	kJ/mol	Joback Method
hvap	72.92	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.426		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1271.87	kPa	Joback Method
rinpol	2086.00		NIST Webbook
rinpol	2086.00		NIST Webbook
tb	760.06	K	Joback Method
tc	941.19	K	Joback Method
tf	420.18	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	824.18	J/molxK	760.06	Joback Method
cpg	841.21	J/molxK	790.25	Joback Method
cpg	857.32	J/molxK	820.44	Joback Method
cpg	872.53	J/molxK	850.63	Joback Method
cpg	886.86	J/molxK	880.81	Joback Method
cpg	900.31	J/molxK	911.00	Joback Method
cpg	912.90	J/molxK	941.19	Joback Method
dvisc	0.0012431	Paxs	420.18	Joback Method

dvisc	0.0005770	Paxs	476.83	Joback Method
dvisc	0.0003153	Paxs	533.47	Joback Method
dvisc	0.0001934	Paxs	590.12	Joback Method
dvisc	0.0001293	Paxs	646.77	Joback Method
dvisc	0.0000922	Paxs	703.41	Joback Method
dvisc	0.0000692	Paxs	760.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391284&Units=SI
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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_cvol:	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

Latest version available from:

<https://www.chemeo.com/cid/88-948-3/Succinic-acid-2-ethylhexyl-hex-5-en-1-yl-ester.pdf>

Generated by Cheméo on 2024-04-23 15:40:29.430207903 +0000 UTC m=+16176078.350785218.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.