

Succinic acid, pent-4-enyl propyl ester

Inchi:	InChI=1S/C12H20O4/c1-3-5-6-10-16-12(14)8-7-11(13)15-9-4-2/h3H,1,4-10H2,2H3
InchiKey:	PBAMUIXLIQFUFN-UHFFFAOYSA-N
Formula:	C12H20O4
SMILES:	C=CCCCOC(=O)CCC(=O)OCCC
Mol. weight [g/mol]:	228.28

Physical Properties

Property code	Value	Unit	Source
gf	-329.84	kJ/mol	Joback Method
hf	-655.18	kJ/mol	Joback Method
hfus	31.13	kJ/mol	Joback Method
hvap	59.95	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.229		Crippen Method
mcvol	190.520	ml/mol	McGowan Method
pc	2000.12	kPa	Joback Method
rinsol	1554.00		NIST Webbook
tb	623.22	K	Joback Method
tc	803.24	K	Joback Method
tf	367.56	K	Joback Method
vc	0.737	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.13	J/molxK	623.22	Joback Method
cpg	508.13	J/molxK	653.22	Joback Method
cpg	521.49	J/molxK	683.23	Joback Method
cpg	534.23	J/molxK	713.23	Joback Method
cpg	546.34	J/molxK	743.23	Joback Method
cpg	557.83	J/molxK	773.24	Joback Method
cpg	568.70	J/molxK	803.24	Joback Method
dvisc	0.0016765	Paxs	367.56	Joback Method
dvisc	0.0009230	Paxs	410.17	Joback Method

dvisc	0.0005686	Paxs	452.78	Joback Method
dvisc	0.0003807	Paxs	495.39	Joback Method
dvisc	0.0002716	Paxs	538.00	Joback Method
dvisc	0.0002036	Paxs	580.61	Joback Method
dvisc	0.0001588	Paxs	623.22	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=U353368&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
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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