

Succinic acid, 8-chlorooctyl hex-5-en-1-yl ester

Inchi:	InChI=1S/C18H31ClO4/c1-2-3-4-10-15-22-17(20)12-13-18(21)23-16-11-8-6-5-7-9-14-19
InchiKey:	BFVSTGCZCBBQOO-UHFFFAOYSA-N
Formula:	C18H31ClO4
SMILES:	C=CCCCCOC(=O)CCC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	346.89

Physical Properties

Property code	Value	Unit	Source
gf	-291.25	kJ/mol	Joback Method
hf	-794.76	kJ/mol	Joback Method
hfus	50.87	kJ/mol	Joback Method
hvap	77.69	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.789		Crippen Method
mcvol	287.300	ml/mol	McGowan Method
pc	1232.01	kPa	Joback Method
rinpol	2518.00		NIST Webbook
rinpol	2518.00		NIST Webbook
tb	797.93	K	Joback Method
tc	983.41	K	Joback Method
tf	465.10	K	Joback Method
vc	1.121	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	854.53	J/molxK	797.93	Joback Method
cpg	870.53	J/molxK	828.84	Joback Method
cpg	885.59	J/molxK	859.76	Joback Method
cpg	899.75	J/molxK	890.67	Joback Method
cpg	913.01	J/molxK	921.58	Joback Method
cpg	925.40	J/molxK	952.50	Joback Method
cpg	936.93	J/molxK	983.41	Joback Method
dvisc	0.0008397	Paxs	465.10	Joback Method

dvisc	0.0004373	Paxs	520.57	Joback Method
dvisc	0.0002582	Paxs	576.04	Joback Method
dvisc	0.0001672	Paxs	631.52	Joback Method
dvisc	0.0001162	Paxs	686.99	Joback Method
dvisc	0.0000852	Paxs	742.46	Joback Method
dvisc	0.0000653	Paxs	797.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391291&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

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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