

Succinic acid, 8-chlorooctyl hexyl ester

Inchi:	InChI=1S/C18H33ClO4/c1-2-3-4-10-15-22-17(20)12-13-18(21)23-16-11-8-6-5-7-9-14-19
InchiKey:	OSANRUGTBBHCED-UHFFFAOYSA-N
Formula:	C18H33ClO4
SMILES:	CCCCCOC(=O)CCC(=O)OCCCCCCCCCI
Mol. weight [g/mol]:	348.90

Physical Properties

Property code	Value	Unit	Source
gf	-379.09	kJ/mol	Joback Method
hf	-920.19	kJ/mol	Joback Method
hfus	52.15	kJ/mol	Joback Method
hvap	78.36	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	5.013		Crippen Method
mvol	291.600	ml/mol	McGowan Method
pc	1196.48	kPa	Joback Method
rinpol	2452.00		NIST Webbook
tb	801.25	K	Joback Method
tc	986.02	K	Joback Method
tf	466.86	K	Joback Method
vc	1.141	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	881.08	J/molxK	801.25	Joback Method
cpg	897.61	J/molxK	832.05	Joback Method
cpg	913.18	J/molxK	862.84	Joback Method
cpg	927.81	J/molxK	893.64	Joback Method
cpg	941.51	J/molxK	924.43	Joback Method
cpg	954.29	J/molxK	955.23	Joback Method
cpg	966.18	J/molxK	986.02	Joback Method
dvisc	0.0008274	Paxs	466.86	Joback Method
dvisc	0.0004253	Paxs	522.59	Joback Method

dvisc	0.0002486	Paxs	578.32	Joback Method
dvisc	0.0001596	Paxs	634.06	Joback Method
dvisc	0.0001101	Paxs	689.79	Joback Method
dvisc	0.0000803	Paxs	745.52	Joback Method
dvisc	0.0000612	Paxs	801.25	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=U349290&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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