

Succinic acid, 8-chlorooctyl pent-4-en-1-yl ester

Inchi:	InChI=1S/C17H29ClO4/c1-2-3-9-14-21-16(19)11-12-17(20)22-15-10-7-5-4-6-8-13-18/h2H
InchiKey:	OAPJSLDFBCKHJO-UHFFFAOYSA-N
Formula:	C17H29ClO4
SMILES:	C=CCCCOC(=O)CCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]:	332.86

Physical Properties

Property code	Value	Unit	Source
gf	-299.67	kJ/mol	Joback Method
hf	-774.12	kJ/mol	Joback Method
hfus	48.28	kJ/mol	Joback Method
hvap	75.46	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.399		Crippen Method
mvol	273.210	ml/mol	McGowan Method
pc	1319.43	kPa	Joback Method
rinpol	2371.00		NIST Webbook
rinpol	2371.00		NIST Webbook
tb	775.05	K	Joback Method
tc	958.92	K	Joback Method
tf	453.83	K	Joback Method
vc	1.065	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.50	J/mol×K	775.05	Joback Method
cpg	812.10	J/mol×K	805.70	Joback Method
cpg	826.81	J/mol×K	836.34	Joback Method
cpg	840.67	J/mol×K	866.99	Joback Method
cpg	853.67	J/mol×K	897.63	Joback Method
cpg	865.85	J/mol×K	928.28	Joback Method
cpg	877.20	J/mol×K	958.92	Joback Method
dvisc	0.0009301	Paxs	453.83	Joback Method

dvisc	0.0004903	Paxs	507.37	Joback Method
dvisc	0.0002921	Paxs	560.90	Joback Method
dvisc	0.0001904	Paxs	614.44	Joback Method
dvisc	0.0001330	Paxs	667.98	Joback Method
dvisc	0.0000979	Paxs	721.51	Joback Method
dvisc	0.0000752	Paxs	775.05	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=U391075&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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