Succinic acid, 8-chlorooctyl trans-hex-3-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: GVZXVMFDMRRAML-ONEGZZNKSA-N

Formula: C18H31ClO4

SMILES: CCC=CCCOC(=O)CCC(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 346.89

Physical Properties

Property code	Value	Unit	Source
gf	-298.87	kJ/mol	Joback Method
hf	-802.97	kJ/mol	Joback Method
hfus	52.35	kJ/mol	Joback Method
hvap	78.32	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.789		Crippen Method
mcvol	287.300	ml/mol	McGowan Method
pc	1240.71	kPa	Joback Method
rinpol	2461.00		NIST Webbook
rinpol	2461.00		NIST Webbook
tb	805.41	K	Joback Method
tc	993.22	K	Joback Method
tf	461.78	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.70	J/mol×K	805.41	Joback Method
cpg	871.68	J/mol×K	836.71	Joback Method
cpg	886.75	J/mol×K	868.01	Joback Method
cpg	900.91	J/mol×K	899.31	Joback Method
cpg	914.21	J/mol×K	930.62	Joback Method
cpg	926.66	J/mol×K	961.92	Joback Method
cpg	938.28	J/mol×K	993.22	Joback Method
dvisc	0.0007679	Pa×s	461.78	Joback Method

dvisc	0.0003850	Pa×s	519.05	Joback Method
dvisc	0.0002214	Pa×s	576.32	Joback Method
dvisc	0.0001407	Pa×s	633.60	Joback Method
dvisc	0.0000964	Pa×s	690.87	Joback Method
dvisc	0.0000700	Pa×s	748.14	Joback Method
dvisc	0.0000532	Pa×s	805.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391123&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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