Succinic acid, 8-chlorooctyl but-3-en-1-yl ester

Inchi: InChI=1S/C16H27ClO4/c1-2-3-13-20-15(18)10-11-16(19)21-14-9-7-5-4-6-8-12-17/h2H,1,
InchiKey: CIQCGKQMTIDLMP-UHFFFAOYSA-N
Formula: C16H27ClO4
SMILES: C=CCCOC(=O)CCC(=O)OCCCCCCCCCl
Mol. weight [g/mol]: 318.84

Physical Properties

Property code	Value	Unit	Source
gf	-308.09	kJ/mol	Joback Method
hf	-753.48	kJ/mol	Joback Method
hfus	45.69	kJ/mol	Joback Method
hvap	73.24	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.008		Crippen Method
mcvol	259.120	ml/mol	McGowan Method
pc	1416.50	kPa	Joback Method
rinpol	2262.00		NIST Webbook
rinpol	2262.00		NIST Webbook
tb	752.17	K	Joback Method
tc	935.07	K	Joback Method
tf	442.56	K	Joback Method
vc	1.010	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.44	J/mol×K	752.17	Joback Method
cpg	807.19	J/mol×K	904.59	Joback Method
cpg	795.25	J/mol×K	874.11	Joback Method
cpg	782.52	J/mol×K	843.62	Joback Method
cpg	768.98	J/mol×K	813.14	Joback Method
cpg	754.63	J/mol×K	782.65	Joback Method
cpg	818.35	J/mol×K	935.07	Joback Method
dvisc	0.0000864	Pa×s	752.17	Joback Method

dvisc	0.0001121	Pa×s	700.57	Joback Method
dvisc	0.0001517	Pa×s	648.97	Joback Method
dvisc	0.0002161	Pa×s	597.37	Joback Method
dvisc	0.0003292	Pa×s	545.76	Joback Method
dvisc	0.0005476	Pa×s	494.16	Joback Method
dvisc	0.0010256	Pa×s	442.56	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=U391201&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