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

Inchi: InChI=1S/C17H29ClO4/c1-15(2)11-14-22-17(20)10-9-16(19)21-13-8-6-4-3-5-7-12-18/h1,

InchiKey: FCOVUAUGPFVYFC-UHFFFAOYSA-N

Formula: C17H29ClO4

SMILES: C=C(C)CCOC(=O)CCC(=O)OCCCCCCCCCl

Mol. weight [g/mol]: 332.86

Physical Properties

Property code	Value	Unit	Source
gf	-308.22	kJ/mol	Joback Method
hf	-783.91	kJ/mol	Joback Method
hfus	46.97	kJ/mol	Joback Method
hvap	75.54	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.399		Crippen Method
mcvol	273.210	ml/mol	McGowan Method
pc	1324.24	kPa	Joback Method
rinpol	2354.00		NIST Webbook
rinpol	2354.00		NIST Webbook
tb	774.93	K	Joback Method
tc	960.14	K	Joback Method
tf	439.87	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.14	J/mol×K	774.93	Joback Method
cpg	811.84	J/mol×K	805.80	Joback Method
cpg	826.65	J/mol×K	836.67	Joback Method
cpg	840.59	J/mol×K	867.53	Joback Method
cpg	853.67	J/mol×K	898.40	Joback Method
cpg	865.92	J/mol×K	929.27	Joback Method
cpg	877.34	J/mol×K	960.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391144&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

Legend

cpg:	Ideal gas heat capacity
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