Succinic acid, 2,2-dichloroethyl dodec-9-yn-1-yl ester

Inchi: InChI=1S/C18H28Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-14-23-17(21)12-13-18(22)24-15-16(19

InchiKey: KFFMKJYVFSGHOQ-UHFFFAOYSA-N

Formula: C18H28Cl2O4

SMILES: CCC#CCCCCCCCCOC(=O)CCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 379.32

Physical Properties

Property code	Value	Unit	Source
gf	-190.66	kJ/mol	Joback Method
hf	-668.91	kJ/mol	Joback Method
hfus	55.94	kJ/mol	Joback Method
hvap	84.51	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.801		Crippen Method
mcvol	295.240	ml/mol	McGowan Method
pc	1312.75	kPa	Joback Method
rinpol	2586.00		NIST Webbook
rinpol	2586.00		NIST Webbook
tb	847.24	K	Joback Method
tc	1047.79	K	Joback Method
tf	587.88	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	859.61	J/mol×K	847.24	Joback Method
cpg	874.40	J/mol×K	880.66	Joback Method
cpg	888.16	J/mol×K	914.09	Joback Method
cpg	900.92	J/mol×K	947.51	Joback Method
cpg	912.69	J/mol×K	980.94	Joback Method
cpg	923.48	J/mol×K	1014.36	Joback Method
cpg	933.31	J/mol×K	1047.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390998&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