Succinic acid, 2,2-dichloroethyl non-5-yn-3-yl ester

Inchi: InChI=1S/C15H22Cl2O4/c1-3-5-6-7-8-12(4-2)21-15(19)10-9-14(18)20-11-13(16)17/h12-1

InchiKey: NSKMRDPOEKYEBA-UHFFFAOYSA-N

Formula: C15H22Cl2O4

SMILES: CCCC#CCC(CC)OC(=O)CCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 337.24

Physical Properties

Property code	Value	Unit	Source
gf	-218.36	kJ/mol	Joback Method
hf	-612.27	kJ/mol	Joback Method
hfus	44.65	kJ/mol	Joback Method
hvap	77.44	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	3.629		Crippen Method
mcvol	252.970	ml/mol	McGowan Method
pc	1647.09	kPa	Joback Method
rinpol	2131.00		NIST Webbook
rinpol	2131.00		NIST Webbook
tb	778.16	K	Joback Method
tc	981.40	K	Joback Method
tf	539.07	K	Joback Method
vc	0.972	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.43	J/mol×K	778.16	Joback Method
cpg	703.45	J/mol×K	812.03	Joback Method
cpg	716.54	J/mol×K	845.91	Joback Method
cpg	728.73	J/mol×K	879.78	Joback Method
cpg	740.01	J/mol×K	913.66	Joback Method
cpg	750.39	J/mol×K	947.53	Joback Method
cpg	759.89	J/mol×K	981.40	Joback Method

Sources

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=U391010&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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