

Succinic acid, 2,2-dichloroethyl 3-phenylpropyl ester

Inchi: InChI=1S/C15H18Cl2O4/c16-13(17)11-21-15(19)9-8-14(18)20-10-4-7-12-5-2-1-3-6-12/h
InchiKey: AILRFBBCUROPLH-UHFFFAOYSA-N
Formula: C15H18Cl2O4
SMILES: O=C(CCC(=O)OCC(Cl)Cl)OCCCc1ccccc1
Mol. weight [g/mol]: 333.21

Physical Properties

Property code	Value	Unit	Source
gf	-306.31	kJ/mol	Joback Method
hf	-642.76	kJ/mol	Joback Method
hfus	39.09	kJ/mol	Joback Method
hvap	77.95	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.289		Crippen Method
mvol	237.810	ml/mol	McGowan Method
pc	1888.72	kPa	Joback Method
rinpol	2350.00		NIST Webbook
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tb	796.28	K	Joback Method
tc	1009.25	K	Joback Method
tf	474.39	K	Joback Method
vc	0.907	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	646.55	J/molxK	796.28	Joback Method
cpg	700.79	J/molxK	973.75	Joback Method
cpg	691.88	J/molxK	938.26	Joback Method
cpg	682.02	J/molxK	902.76	Joback Method
cpg	671.20	J/molxK	867.27	Joback Method
cpg	659.38	J/molxK	831.77	Joback Method
cpg	708.78	J/molxK	1009.25	Joback Method
dvisc	0.0000756	Paxs	796.28	Joback Method

dvisc	0.0000981	Paxs	742.63	Joback Method
dvisc	0.0001326	Paxs	688.98	Joback Method
dvisc	0.0001886	Paxs	635.34	Joback Method
dvisc	0.0002862	Paxs	581.69	Joback Method
dvisc	0.0004728	Paxs	528.04	Joback Method
dvisc	0.0008749	Paxs	474.39	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=U389726&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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