

Succinic acid, 2,2-dichloroethyl 10-chlorodecyl ester

Inchi:	InChI=1S/C16H27Cl3O4/c17-11-7-5-3-1-2-4-6-8-12-22-15(20)9-10-16(21)23-13-14(18)19
InchiKey:	LYBYCFCUTQGKHI-UHFFFAOYSA-N
Formula:	C16H27Cl3O4
SMILES:	O=C(CCC(=O)OCC(Cl)Cl)OCCCCCCCCCCC
Mol. weight [g/mol]:	389.74

Physical Properties

Property code	Value	Unit	Source
gf	-422.23	kJ/mol	Joback Method
hf	-915.67	kJ/mol	Joback Method
hfus	51.84	kJ/mol	Joback Method
hvap	82.29	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	5.016		Crippen Method
mcvol	287.900	ml/mol	McGowan Method
pc	1308.01	kPa	Joback Method
rinpol	2640.00		NIST Webbook
rinpol	2640.00		NIST Webbook
tb	829.91	K	Joback Method
tc	1023.93	K	Joback Method
tf	489.16	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	821.93	J/molxK	829.91	Joback Method
cpg	882.63	J/molxK	991.59	Joback Method
cpg	872.31	J/molxK	959.25	Joback Method
cpg	861.09	J/molxK	926.92	Joback Method
cpg	848.97	J/molxK	894.58	Joback Method
cpg	835.92	J/molxK	862.25	Joback Method
cpg	892.08	J/molxK	1023.93	Joback Method
dvisc	0.0000550	Paxs	829.91	Joback Method

dvisc	0.0000724	Paxs	773.12	Joback Method
dvisc	0.0000995	Paxs	716.33	Joback Method
dvisc	0.0001445	Paxs	659.53	Joback Method
dvisc	0.0002252	Paxs	602.74	Joback Method
dvisc	0.0003849	Paxs	545.95	Joback Method
dvisc	0.0007450	Paxs	489.16	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=U390408&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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