

Succinic acid, 2,4,6-trichlorophenyl cyclopentyl ester

Inchi:	InChI=1S/C15H15Cl3O4/c16-9-7-11(17)15(12(18)8-9)22-14(20)6-5-13(19)21-10-3-1-2-4
InchiKey:	LZXGIVFGTIACRL-UHFFFAOYSA-N
Formula:	C15H15Cl3O4
SMILES:	O=C(CCC(=O)OC1CCCC1)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	365.64

Physical Properties

Property code	Value	Unit	Source
gf	-308.14	kJ/mol	Joback Method
hf	-627.15	kJ/mol	Joback Method
hfus	39.58	kJ/mol	Joback Method
hvap	84.97	kJ/mol	Joback Method
log10ws	-5.64		Crippen Method
logp	4.818		Crippen Method
mcvol	239.190	ml/mol	McGowan Method
pc	2045.61	kPa	Joback Method
rinpol	2528.00		NIST Webbook
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tb	864.37	K	Joback Method
tc	1100.84	K	Joback Method
tf	567.77	K	Joback Method
vc	0.903	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.21	J/molxK	864.37	Joback Method
cpg	665.02	J/molxK	903.78	Joback Method
cpg	675.59	J/molxK	943.19	Joback Method
cpg	684.94	J/molxK	982.60	Joback Method
cpg	693.11	J/molxK	1022.01	Joback Method
cpg	700.10	J/molxK	1061.43	Joback Method
cpg	705.94	J/molxK	1100.84	Joback Method
dvisc	0.0005865	Paxs	567.77	Joback Method

dvisc	0.0003971	Paxs	617.20	Joback Method
dvisc	0.0002849	Paxs	666.64	Joback Method
dvisc	0.0002140	Paxs	716.07	Joback Method
dvisc	0.0001668	Paxs	765.50	Joback Method
dvisc	0.0001340	Paxs	814.94	Joback Method
dvisc	0.0001104	Paxs	864.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391384&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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