

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

Inchi:	InChI=1S/C17H12Cl4O4/c18-11-3-1-10(2-4-11)9-24-15(22)5-6-16(23)25-17-13(20)7-12(
InchiKey:	YDOCGTSXTJFLKZ-UHFFFAOYSA-N
Formula:	C17H12Cl4O4
SMILES:	O=C(CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCc1ccc(Cl)cc1
Mol. weight [g/mol]:	422.09

Physical Properties

Property code	Value	Unit	Source
gf	-237.00	kJ/mol	Joback Method
hf	-519.59	kJ/mol	Joback Method
hfus	48.67	kJ/mol	Joback Method
hvap	96.49	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	5.729		Crippen Method
mcvol	266.710	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
rinsol	3016.00		NIST Webbook
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tb	963.94	K	Joback Method
tc	1208.81	K	Joback Method
tf	648.27	K	Joback Method
vc	1.016	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.12	J/molxK	963.94	Joback Method
cpg	696.16	J/molxK	1004.75	Joback Method
cpg	702.98	J/molxK	1045.56	Joback Method
cpg	708.60	J/molxK	1086.37	Joback Method
cpg	713.06	J/molxK	1127.19	Joback Method
cpg	716.37	J/molxK	1168.00	Joback Method
cpg	718.54	J/molxK	1208.81	Joback Method
dvisc	0.0002501	Paxs	648.27	Joback Method

dvisc	0.0001728	Paxs	700.88	Joback Method
dvisc	0.0001257	Paxs	753.49	Joback Method
dvisc	0.0000953	Paxs	806.11	Joback Method
dvisc	0.0000748	Paxs	858.72	Joback Method
dvisc	0.0000603	Paxs	911.33	Joback Method
dvisc	0.0000498	Paxs	963.94	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=U389683&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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