

Succinic acid, 4-chloro-3-methylphenyl 4-chloro-2-methoxyphenyl ester

Inchi:	InChI=1S/C18H16Cl2O5/c1-11-9-13(4-5-14(11)20)24-17(21)7-8-18(22)25-15-6-3-12(19)
InchiKey:	JEASZMFPGBJMMY-UHFFFAOYSA-N
Formula:	C18H16Cl2O5
SMILES:	COc1cc(Cl)ccc1OC(=O)CCC(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]:	383.22

Physical Properties

Property code	Value	Unit	Source
gf	-309.72	kJ/mol	Joback Method
hf	-640.97	kJ/mol	Joback Method
hfus	44.06	kJ/mol	Joback Method
hvap	92.35	kJ/mol	Joback Method
log10ws	-5.71		Crippen Method
logp	4.602		Crippen Method
mcvol	262.190	ml/mol	McGowan Method
pc	1821.61	kPa	Joback Method
rinpol	2923.00		NIST Webbook
rinpol	2923.00		NIST Webbook
tb	934.38	K	Joback Method
tc	1169.70	K	Joback Method
tf	621.93	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.74	J/molxK	934.38	Joback Method
cpg	742.82	J/molxK	973.60	Joback Method
cpg	751.52	J/molxK	1012.82	Joback Method
cpg	758.84	J/molxK	1052.04	Joback Method
cpg	764.76	J/molxK	1091.26	Joback Method
cpg	769.29	J/molxK	1130.48	Joback Method
cpg	772.42	J/molxK	1169.70	Joback Method
dvisc	0.0002290	Paxs	621.93	Joback Method

dvisc	0.0001564	Paxs	674.00	Joback Method
dvisc	0.0001129	Paxs	726.08	Joback Method
dvisc	0.0000851	Paxs	778.15	Joback Method
dvisc	0.0000664	Paxs	830.23	Joback Method
dvisc	0.0000534	Paxs	882.30	Joback Method
dvisc	0.0000440	Paxs	934.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390944&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

Latest version available from:

<https://www.chemeo.com/cid/122-797-2/Succinic-acid-4-chloro-3-methylphenyl-4-chloro-2-methoxyphenyl-ester.pdf>

Generated by Cheméo on 2024-04-28 23:34:47.123990004 +0000 UTC m=+16636536.044567316.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.