

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

Inchi:	InChI=1S/C18H15Cl3O5/c1-24-13-4-2-11(3-5-13)10-25-16(22)6-7-17(23)26-18-14(20)8-
InchiKey:	MXDDIBHORGYGDM-UHFFFAOYSA-N
Formula:	C18H15Cl3O5
SMILES:	COc1ccc(COC(=O)CCC(=O)Oc2c(Cl)cc(Cl)cc2Cl)cc1
Mol. weight [g/mol]:	417.67

Physical Properties

Property code	Value	Unit	Source
gf	-321.65	kJ/mol	Joback Method
hf	-656.71	kJ/mol	Joback Method
hfus	48.26	kJ/mol	Joback Method
hvap	96.74	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.084		Crippen Method
mcvol	274.430	ml/mol	McGowan Method
pc	1765.41	kPa	Joback Method
rinpol	3040.00		NIST Webbook
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tb	971.81	K	Joback Method
tc	1210.69	K	Joback Method
tf	651.85	K	Joback Method
vc	1.040	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.87	J/molxK	971.81	Joback Method
cpg	779.80	J/molxK	1170.87	Joback Method
cpg	776.83	J/molxK	1131.06	Joback Method
cpg	772.45	J/molxK	1091.25	Joback Method
cpg	766.66	J/molxK	1051.44	Joback Method
cpg	759.47	J/molxK	1011.62	Joback Method
cpg	781.37	J/molxK	1210.69	Joback Method
dvisc	0.0000376	Paxs	971.81	Joback Method

dvisc	0.0000456	Paxs	918.48	Joback Method
dvisc	0.0000566	Paxs	865.16	Joback Method
dvisc	0.0000724	Paxs	811.83	Joback Method
dvisc	0.0000959	Paxs	758.50	Joback Method
dvisc	0.0001325	Paxs	705.18	Joback Method
dvisc	0.0001929	Paxs	651.85	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=U389697&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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