Succinic acid, 2,4,6-trichlorophenyl 5-methoxy-3-methylpent-2-yl ester

Inchi: InChI=1S/C17H21Cl3O5/c1-10(6-7-23-3)11(2)24-15(21)4-5-16(22)25-17-13(19)8-12(18)9

InchiKey: CSFSODINFHGAMS-UHFFFAOYSA-N

Formula: C17H21Cl3O5

SMILES: COCCC(C)C(C)OC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 411.70

Physical Properties

Property code	Value	Unit	Source
gf	-437.73	kJ/mol	Joback Method
hf	-871.69	kJ/mol	Joback Method
hfus	44.97	kJ/mol	Joback Method
hvap	90.80	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.937		Crippen Method
mcvol	284.100	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinpol	2615.00		NIST Webbook
rinpol	2615.00		NIST Webbook
tb	916.39	K	Joback Method
tc	1135.91	K	Joback Method
tf	571.64	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.15	J/mol×K	916.39	Joback Method
cpg	815.46	J/mol×K	952.98	Joback Method
cpg	825.52	J/mol×K	989.56	Joback Method
cpg	834.31	J/mol×K	1026.15	Joback Method
cpg	841.84	J/mol×K	1062.74	Joback Method
cpg	848.09	J/mol×K	1099.32	Joback Method
cpg	853.07	J/mol×K	1135.91	Joback Method
dvisc	0.0002886	Pa×s	571.64	Joback Method

dvisc	0.0001720	Pa×s	629.10	Joback Method
dvisc	0.0001118	Pa×s	686.56	Joback Method
dvisc	0.0000777	Pa×s	744.01	Joback Method
dvisc	0.0000568	Pa×s	801.47	Joback Method
dvisc	0.0000434	Pa×s	858.93	Joback Method
dvisc	0.0000342	Pa×s	916.39	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=U389667&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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