Succinic acid, monochloride 2-chloro-5-methylphenyl ester

Inchi: InChI=1S/C11H10Cl2O3/c1-7-2-3-8(12)9(6-7)16-11(15)5-4-10(13)14/h2-3,6H,4-5H2,1H3

InchiKey: GCFIYXKATZKXNR-UHFFFAOYSA-N

Formula: C11H10Cl2O3

SMILES: Cc1ccc(Cl)c(OC(=O)CCC(=O)Cl)c1

Mol. weight [g/mol]: 261.10

Physical Properties

Property code	Value	Unit	Source
gf	-251.81	kJ/mol	Joback Method
hf	-445.64	kJ/mol	Joback Method
hfus	30.29	kJ/mol	Joback Method
hvap	68.35	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.099		Crippen Method
mcvol	175.580	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpol	1818.00		NIST Webbook
rinpol	1818.00		NIST Webbook
tb	692.74	K	Joback Method
tc	917.95	K	Joback Method
tf	447.12	K	Joback Method
vc	0.671	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.63	J/mol×K	692.74	Joback Method
cpg	419.47	J/mol×K	730.28	Joback Method
cpg	429.53	J/mol×K	767.81	Joback Method
cpg	438.83	J/mol×K	805.35	Joback Method
cpg	447.37	J/mol×K	842.88	Joback Method
cpg	455.19	J/mol×K	880.42	Joback Method
cpg	462.27	J/mol×K	917.95	Joback Method
dvisc	0.0010688	Pa×s	447.12	Joback Method

dvisc	0.0007029	Pa×s	488.06	Joback Method
dvisc	0.0004932	Pa×s	528.99	Joback Method
dvisc	0.0003642	Pa×s	569.93	Joback Method
dvisc	0.0002800	Pa×s	610.87	Joback Method
dvisc	0.0002226	Pa×s	651.80	Joback Method
dvisc	0.0001817	Pa×s	692.74	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=U353620&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