

Succinic acid, butyl 2,3,5-trichlorophenyl ester

Inchi:	InChI=1S/C14H15Cl3O4/c1-2-3-6-20-12(18)4-5-13(19)21-11-8-9(15)7-10(16)14(11)17/h
InchiKey:	IFEDMJNUTFOCNH-UHFFFAOYSA-N
Formula:	C14H15Cl3O4
SMILES:	CCCCOC(=O)CCC(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	353.62

Physical Properties

Property code	Value	Unit	Source
gf	-353.11	kJ/mol	Joback Method
hf	-666.99	kJ/mol	Joback Method
hfus	43.05	kJ/mol	Joback Method
hvap	82.49	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.676		Crippen Method
mvol	235.960	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinpol	2313.00		NIST Webbook
rinpol	2313.00		NIST Webbook
tb	826.21	K	Joback Method
tc	1043.90	K	Joback Method
tf	545.60	K	Joback Method
vc	0.906	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.81	J/mol×K	826.21	Joback Method
cpg	620.76	J/mol×K	862.49	Joback Method
cpg	630.78	J/mol×K	898.77	Joback Method
cpg	639.87	J/mol×K	935.06	Joback Method
cpg	648.02	J/mol×K	971.34	Joback Method
cpg	655.24	J/mol×K	1007.62	Joback Method
cpg	661.54	J/mol×K	1043.90	Joback Method
dvisc	0.0004707	Paxs	545.60	Joback Method

dvisc	0.0003158	Paxs	592.37	Joback Method
dvisc	0.0002246	Paxs	639.14	Joback Method
dvisc	0.0001673	Paxs	685.90	Joback Method
dvisc	0.0001294	Paxs	732.67	Joback Method
dvisc	0.0001033	Paxs	779.44	Joback Method
dvisc	0.0000845	Paxs	826.21	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=U349608&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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