

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

Inchi:	InChI=1S/C14H15Cl3O4/c1-8(2)7-20-12(18)3-4-13(19)21-11-6-9(15)5-10(16)14(11)17/h5
InchiKey:	VSZGGQBPIKEDPE-UHFFFAOYSA-N
Formula:	C14H15Cl3O4
SMILES:	CC(C)COC(=O)CCC(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	353.62

Physical Properties

Property code	Value	Unit	Source
gf	-355.55	kJ/mol	Joback Method
hf	-672.27	kJ/mol	Joback Method
hfus	39.53	kJ/mol	Joback Method
hvap	82.10	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.532		Crippen Method
mcvol	235.960	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinsol	2257.00		NIST Webbook
tb	825.77	K	Joback Method
tc	1046.49	K	Joback Method
tf	530.60	K	Joback Method
vc	0.900	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.41	J/molxK	825.77	Joback Method
cpg	621.51	J/molxK	862.56	Joback Method
cpg	631.62	J/molxK	899.34	Joback Method
cpg	640.77	J/molxK	936.13	Joback Method
cpg	648.94	J/molxK	972.92	Joback Method
cpg	656.15	J/molxK	1009.70	Joback Method
cpg	662.39	J/molxK	1046.49	Joback Method
dvisc	0.0005101	Paxs	530.60	Joback Method
dvisc	0.0003261	Paxs	579.80	Joback Method

dvisc	0.0002236	Paxs	628.99	Joback Method
dvisc	0.0001620	Paxs	678.18	Joback Method
dvisc	0.0001226	Paxs	727.38	Joback Method
dvisc	0.0000961	Paxs	776.58	Joback Method
dvisc	0.0000775	Paxs	825.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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