Succinic acid, 3-methylbut-2-yl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C15H17Cl3O4/c1-8(2)9(3)21-14(19)4-5-15(20)22-13-7-11(17)10(16)6-12(13)18

InchiKey: KNBPUCOZXXGHOB-UHFFFAOYSA-N

Formula: C15H17Cl3O4

SMILES: CC(C)C(C)OC(=O)CCC(=O)Oc1cc(Cl)c(Cl)cc1Cl

Mol. weight [g/mol]: 367.65

Physical Properties

Property code	Value	Unit	Source
gf	-349.57	kJ/mol	Joback Method
hf	-698.19	kJ/mol	Joback Method
hfus	38.60	kJ/mol	Joback Method
hvap	83.94	kJ/mol	Joback Method
log10ws	-5.50		Crippen Method
logp	4.920		Crippen Method
mcvol	250.050	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	2293.00		NIST Webbook
rinpol	2293.00		NIST Webbook
tb	848.21	K	Joback Method
tc	1069.88	K	Joback Method
tf	526.87	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.82	J/mol×K	848.21	Joback Method
cpg	712.96	J/mol×K	1032.93	Joback Method
cpg	705.62	J/mol×K	995.99	Joback Method
cpg	697.25	J/mol×K	959.04	Joback Method
cpg	687.83	J/mol×K	922.10	Joback Method
cpg	677.35	J/mol×K	885.15	Joback Method
cpg	719.26	J/mol×K	1069.88	Joback Method
dvisc	0.0000617	Pa×s	848.21	Joback Method

dvisc	0.0000779	Pa×s	794.65	Joback Method
dvisc	0.0001016	Pa×s	741.10	Joback Method
dvisc	0.0001383	Pa×s	687.54	Joback Method
dvisc	0.0001982	Pa×s	633.98	Joback Method
dvisc	0.0003035	Pa×s	580.43	Joback Method
dvisc	0.0005069	Pa×s	526.87	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=U389962&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