

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

Inchi:	InChI=1S/C16H19Cl3O4/c1-4-13(9(2)3)22-15(20)5-6-16(21)23-14-8-11(18)10(17)7-12(14)
InchiKey:	FRKGZYCNYSXNM-UHFFFAOYSA-N
Formula:	C16H19Cl3O4
SMILES:	CCC(OC(=O)CCC(=O)Oc1cc(Cl)c(Cl)cc1Cl)C(C)C
Mol. weight [g/mol]:	381.68

Physical Properties

Property code	Value	Unit	Source
gf	-341.15	kJ/mol	Joback Method
hf	-718.83	kJ/mol	Joback Method
hfus	41.19	kJ/mol	Joback Method
hvap	86.16	kJ/mol	Joback Method
log10ws	-5.92		Crippen Method
logp	5.310		Crippen Method
mvol	264.140	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	2368.00		NIST Webbook
rinpol	2368.00		NIST Webbook
tb	871.09	K	Joback Method
tc	1091.17	K	Joback Method
tf	538.14	K	Joback Method
vc	1.006	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.52	J/molxK	871.09	Joback Method
cpg	733.29	J/molxK	907.77	Joback Method
cpg	743.97	J/molxK	944.45	Joback Method
cpg	753.55	J/molxK	981.13	Joback Method
cpg	762.06	J/molxK	1017.81	Joback Method
cpg	769.49	J/molxK	1054.49	Joback Method
cpg	775.86	J/molxK	1091.17	Joback Method
dvisc	0.0004572	Paxs	538.14	Joback Method

dvisc	0.0002705	Paxs	593.63	Joback Method
dvisc	0.0001750	Paxs	649.12	Joback Method
dvisc	0.0001213	Paxs	704.62	Joback Method
dvisc	0.0000887	Paxs	760.11	Joback Method
dvisc	0.0000676	Paxs	815.60	Joback Method
dvisc	0.0000534	Paxs	871.09	Joback Method

Sources

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=U389963&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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