

Succinic acid, 2,4,6-trichlorophenyl tetrahydrofurfuryl ester

Inchi:	InChI=1S/C15H15Cl3O5/c16-9-6-11(17)15(12(18)7-9)23-14(20)4-3-13(19)22-8-10-2-1-5
InchiKey:	JKDJEJNKXLVEQV-UHFFFAOYSA-N
Formula:	C15H15Cl3O5
SMILES:	O=C(CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCC1CCCO1
Mol. weight [g/mol]:	381.64

Physical Properties

Property code	Value	Unit	Source
gf	-394.26	kJ/mol	Joback Method
hf	-759.15	kJ/mol	Joback Method
hfus	47.56	kJ/mol	Joback Method
hvap	89.48	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	4.055		Crippen Method
mcvol	245.060	ml/mol	McGowan Method
pc	2029.06	kPa	Joback Method
rinpol	2707.00		NIST Webbook
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tb	891.32	K	Joback Method
tc	1126.12	K	Joback Method
tf	594.34	K	Joback Method
vc	0.924	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	680.95	J/molxK	891.32	Joback Method
cpg	723.33	J/molxK	1086.99	Joback Method
cpg	717.25	J/molxK	1047.86	Joback Method
cpg	709.99	J/molxK	1008.72	Joback Method
cpg	701.53	J/molxK	969.59	Joback Method
cpg	691.86	J/molxK	930.45	Joback Method
cpg	728.24	J/molxK	1126.12	Joback Method
dvisc	0.0000947	Paxs	891.32	Joback Method

dvisc	0.0001153	Paxs	841.82	Joback Method
dvisc	0.0001440	Paxs	792.33	Joback Method
dvisc	0.0001852	Paxs	742.83	Joback Method
dvisc	0.0002468	Paxs	693.33	Joback Method
dvisc	0.0003439	Paxs	643.84	Joback Method
dvisc	0.0005063	Paxs	594.34	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U390727&Units=SI

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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