

Succinic acid, di(2,4,5-trichlorophenyl) ester

Inchi: InChI=1S/C16H8Cl6O4/c17-7-3-11(21)13(5-9(7)19)25-15(23)1-2-16(24)26-14-6-10(20)8
InchiKey: BRNHDLCBURZOCR-UHFFFAOYSA-N
Formula: C16H8Cl6O4
SMILES: O=C(CCC(=O)Oc1cc(Cl)c(Cl)cc1Cl)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 476.95

Physical Properties

Property code	Value	Unit	Source
gf	-288.54	kJ/mol	Joback Method
hf	-553.37	kJ/mol	Joback Method
hfus	53.70	kJ/mol	Joback Method
hvap	104.36	kJ/mol	Joback Method
log10ws	-7.86		Crippen Method
logp	6.898		Crippen Method
mcvol	277.100	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	3200.00		NIST Webbook
rinpol	3200.00		NIST Webbook
tb	1025.88	K	Joback Method
tc	1280.42	K	Joback Method
tf	721.88	K	Joback Method
vc	1.058	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	657.78	J/mol×K	1025.88	Joback Method
cpg	662.72	J/mol×K	1068.30	Joback Method
cpg	666.41	J/mol×K	1110.73	Joback Method
cpg	668.86	J/mol×K	1153.15	Joback Method
cpg	670.07	J/mol×K	1195.57	Joback Method
cpg	670.03	J/mol×K	1238.00	Joback Method
cpg	668.76	J/mol×K	1280.42	Joback Method
dvisc	0.0001712	Paxs	721.88	Joback Method

dvisc	0.0001264	Paxs	772.55	Joback Method
dvisc	0.0000968	Paxs	823.21	Joback Method
dvisc	0.0000765	Paxs	873.88	Joback Method
dvisc	0.0000621	Paxs	924.55	Joback Method
dvisc	0.0000514	Paxs	975.21	Joback Method
dvisc	0.0000434	Paxs	1025.88	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=U389978&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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