

Glutaric acid, di(3-chlorophenyl) ester

Inchi:	InChI=1S/C17H14Cl2O4/c18-12-4-1-6-14(10-12)22-16(20)8-3-9-17(21)23-15-7-2-5-13(19)
InchiKey:	BRMYXAURHKUSRS-UHFFFAOYSA-N
Formula:	C17H14Cl2O4
SMILES:	O=C(CCCC(=O)Oc1cccc(Cl)c1)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	353.20

Physical Properties

Property code	Value	Unit	Source
gf	-193.88	kJ/mol	Joback Method
hf	-465.17	kJ/mol	Joback Method
hfus	41.06	kJ/mol	Joback Method
hvap	86.39	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.675		Crippen Method
mcvol	242.230	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinqol	2803.00		NIST Webbook
tb	879.12	K	Joback Method
tc	1116.93	K	Joback Method
tf	563.39	K	Joback Method
vc	0.917	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.24	J/molxK	879.12	Joback Method
cpg	698.12	J/molxK	1077.30	Joback Method
cpg	691.83	J/molxK	1037.66	Joback Method
cpg	684.43	J/molxK	998.03	Joback Method
cpg	675.88	J/molxK	958.39	Joback Method
cpg	666.17	J/molxK	918.76	Joback Method
cpg	703.34	J/molxK	1116.93	Joback Method
dvisc	0.0000651	Paxs	879.12	Joback Method
dvisc	0.0000807	Paxs	826.50	Joback Method

dvisc	0.0001029	Paxs	773.88	Joback Method
dvisc	0.0001359	Paxs	721.25	Joback Method
dvisc	0.0001876	Paxs	668.63	Joback Method
dvisc	0.0002737	Paxs	616.01	Joback Method
dvisc	0.0004284	Paxs	563.39	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=U358825&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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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