

Glutaric acid, 2,4,6-trichlorophenyl 2,4-dichlorophenyl ester

Inchi:	InChI=1S/C17H11Cl5O4/c18-9-4-5-14(11(20)6-9)25-15(23)2-1-3-16(24)26-17-12(21)7-10
InchiKey:	IUKCCWJOFBLWIU-UHFFFAOYSA-N
Formula:	C17H11Cl5O4
SMILES:	O=C(CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	456.53

Physical Properties

Property code	Value	Unit	Source
gf	-258.56	kJ/mol	Joback Method
hf	-546.80	kJ/mol	Joback Method
hfus	52.48	kJ/mol	Joback Method
hvap	101.53	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	6.635		Crippen Method
mvol	278.950	ml/mol	McGowan Method
pc	1801.56	kPa	Joback Method
rinpol	3174.00		NIST Webbook
rinpol	3174.00		NIST Webbook
tb	1006.35	K	Joback Method
tc	1255.15	K	Joback Method
tf	690.71	K	Joback Method
vc	1.065	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	701.63	J/molxK	1006.35	Joback Method
cpg	708.20	J/molxK	1047.82	Joback Method
cpg	713.54	J/molxK	1089.28	Joback Method
cpg	717.64	J/molxK	1130.75	Joback Method
cpg	720.53	J/molxK	1172.22	Joback Method
cpg	722.23	J/molxK	1213.68	Joback Method
cpg	722.75	J/molxK	1255.15	Joback Method
dvisc	0.0001947	Paxs	690.71	Joback Method

dvisc	0.0001386	Paxs	743.32	Joback Method
dvisc	0.0001032	Paxs	795.92	Joback Method
dvisc	0.0000797	Paxs	848.53	Joback Method
dvisc	0.0000635	Paxs	901.14	Joback Method
dvisc	0.0000518	Paxs	953.74	Joback Method
dvisc	0.0000432	Paxs	1006.35	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=U391858&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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