

Glutaric acid, ethyl 2,3,4,5-tetrachlorophenyl ester

Inchi:	InChI=1S/C13H12Cl4O4/c1-2-20-9(18)4-3-5-10(19)21-8-6-7(14)11(15)13(17)12(8)16/h6
InchiKey:	GPMDDCDJPPLGRN-UHFFFAOYSA-N
Formula:	C13H12Cl4O4
SMILES:	CCOC(=O)CCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	374.04

Physical Properties

Property code	Value	Unit	Source
gf	-383.09	kJ/mol	Joback Method
hf	-673.56	kJ/mol	Joback Method
hfus	44.27	kJ/mol	Joback Method
hvap	85.31	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	4.939		Crippen Method
mvol	234.110	ml/mol	McGowan Method
pc	1973.55	kPa	Joback Method
rinpol	2459.00		NIST Webbook
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tb	845.74	K	Joback Method
tc	1069.58	K	Joback Method
tf	576.77	K	Joback Method
vc	0.899	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.46	J/molxK	845.74	Joback Method
cpg	583.87	J/molxK	883.05	Joback Method
cpg	592.38	J/molxK	920.35	Joback Method
cpg	599.96	J/molxK	957.66	Joback Method
cpg	606.62	J/molxK	994.96	Joback Method
cpg	612.34	J/molxK	1032.27	Joback Method
cpg	617.13	J/molxK	1069.58	Joback Method
dvisc	0.0003959	Paxs	576.77	Joback Method

dvisc	0.0002795	Paxs	621.60	Joback Method
dvisc	0.0002067	Paxs	666.43	Joback Method
dvisc	0.0001589	Paxs	711.25	Joback Method
dvisc	0.0001260	Paxs	756.08	Joback Method
dvisc	0.0001025	Paxs	800.91	Joback Method
dvisc	0.0000852	Paxs	845.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360746&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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