

Glutaric acid, propyl 3,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C14H15Cl3O4/c1-2-6-20-12(18)4-3-5-13(19)21-9-7-10(15)14(17)11(16)8-9/h7-
InchiKey:	UDYZWAASVIUOKU-UHFFFAOYSA-N
Formula:	C14H15Cl3O4
SMILES:	CCCOC(=O)CCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
Mol. weight [g/mol]:	353.62

Physical Properties

Property code	Value	Unit	Source
gf	-353.11	kJ/mol	Joback Method
hf	-666.99	kJ/mol	Joback Method
hfus	43.05	kJ/mol	Joback Method
hvap	82.49	kJ/mol	Joback Method
log10ws	-5.21		Crippen Method
logp	4.676		Crippen Method
mcvol	235.960	ml/mol	McGowan Method
pc	1898.60	kPa	Joback Method
rinqol	2449.00		NIST Webbook
tb	826.21	K	Joback Method
tc	1043.90	K	Joback Method
tf	545.60	K	Joback Method
vc	0.906	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.81	J/molxK	826.21	Joback Method
cpg	620.76	J/molxK	862.49	Joback Method
cpg	630.78	J/molxK	898.77	Joback Method
cpg	639.87	J/molxK	935.06	Joback Method
cpg	648.02	J/molxK	971.34	Joback Method
cpg	655.24	J/molxK	1007.62	Joback Method
cpg	661.54	J/molxK	1043.90	Joback Method
dvisc	0.0004707	Paxs	545.60	Joback Method
dvisc	0.0003158	Paxs	592.37	Joback Method

dvisc	0.0002246	Paxs	639.14	Joback Method
dvisc	0.0001673	Paxs	685.90	Joback Method
dvisc	0.0001294	Paxs	732.67	Joback Method
dvisc	0.0001033	Paxs	779.44	Joback Method
dvisc	0.0000845	Paxs	826.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359142&Units=SI
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

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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