Glutaric acid, ethyl 2,3,5-trichlorophenyl ester

Inchi: InChI=1S/C13H13Cl3O4/c1-2-19-11(17)4-3-5-12(18)20-10-7-8(14)6-9(15)13(10)16/h6-7H
InchiKey: IRKWAFVXFGZMOI-UHFFFAOYSA-N
Formula: C13H13Cl3O4
SMILES: CCOC(=O)CCCC(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 339.60

Physical Properties

Property code	Value	Unit	Source
gf	-361.53	kJ/mol	Joback Method
hf	-646.35	kJ/mol	Joback Method
hfus	40.46	kJ/mol	Joback Method
hvap	80.26	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	4.286		Crippen Method
mcvol	221.870	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	2567.00		NIST Webbook
rinpol	2567.00		NIST Webbook
tb	803.33	K	Joback Method
tc	1023.24	K	Joback Method
tf	534.33	K	Joback Method
vc	0.851	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.95	J/mol×K	803.33	Joback Method
cpg	566.52	J/mol×K	839.98	Joback Method
cpg	576.20	J/mol×K	876.63	Joback Method
cpg	584.99	J/mol×K	913.28	Joback Method
cpg	592.88	J/mol×K	949.93	Joback Method
cpg	599.88	J/mol×K	986.59	Joback Method
cpg	605.98	J/mol×K	1023.24	Joback Method
dvisc	0.0005145	Pa×s	534.33	Joback Method

dvisc	0.0003497	Pa×s	579.16	Joback Method
dvisc	0.0002513	Pa×s	624.00	Joback Method
dvisc	0.0001887	Pa×s	668.83	Joback Method
dvisc	0.0001469	Pa×s	713.66	Joback Method
dvisc	0.0001178	Pa×s	758.50	Joback Method
dvisc	0.0000969	Pa×s	803.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359117&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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