

Glutaric acid, ethyl 2,3,6-trichlorophenyl ester

Inchi:	InChI=1S/C13H13Cl3O4/c1-2-19-10(17)4-3-5-11(18)20-13-9(15)7-6-8(14)12(13)16/h6-7
InchiKey:	CPCYVIXDQNIJZR-UHFFFAOYSA-N
Formula:	C13H13Cl3O4
SMILES:	CCOC(=O)CCCC(=O)Oc1c(Cl)ccc(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
mvol	221.870	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	2272.00		NIST Webbook
tb	803.33	K	Joback Method
tc	1023.24	K	Joback Method
tf	534.33	K	Joback Method
vc	0.851	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	555.95	J/molxK	803.33	Joback Method
cpg	566.52	J/molxK	839.98	Joback Method
cpg	576.20	J/molxK	876.63	Joback Method
cpg	584.99	J/molxK	913.28	Joback Method
cpg	592.88	J/molxK	949.93	Joback Method
cpg	599.88	J/molxK	986.59	Joback Method
cpg	605.98	J/molxK	1023.24	Joback Method
dvisc	0.0005145	Paxs	534.33	Joback Method
dvisc	0.0003497	Paxs	579.16	Joback Method

dvisc	0.0002513	Paxs	624.00	Joback Method
dvisc	0.0001887	Paxs	668.83	Joback Method
dvisc	0.0001469	Paxs	713.66	Joback Method
dvisc	0.0001178	Paxs	758.50	Joback Method
dvisc	0.0000969	Paxs	803.33	Joback Method

Sources

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=U359240&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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