

Glutaric acid, 2,2-dichloroethyl 3-chlorophenyl ester

Inchi:	InChI=1S/C13H13Cl3O4/c14-9-3-1-4-10(7-9)20-13(18)6-2-5-12(17)19-8-11(15)16/h1,3-4
InchiKey:	LWSQGNIVZWGJIE-UHFFFAOYSA-N
Formula:	C13H13Cl3O4
SMILES:	O=C(CCCC(=O)Oc1cccc(Cl)c1)OCC(Cl)Cl
Mol. weight [g/mol]:	339.60

Physical Properties

Property code	Value	Unit	Source
gf	-344.71	kJ/mol	Joback Method
hf	-628.69	kJ/mol	Joback Method
hfus	37.72	kJ/mol	Joback Method
hvap	78.55	kJ/mol	Joback Method
log10ws	-4.34		Crippen Method
logp	3.763		Crippen Method
mcvol	221.870	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpola	2318.00		NIST Webbook
rinpola	2318.00		NIST Webbook
tb	792.93	K	Joback Method
tc	1014.67	K	Joback Method
tf	494.29	K	Joback Method
vc	0.845	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.79	J/molxK	792.93	Joback Method
cpg	570.68	J/molxK	829.89	Joback Method
cpg	580.63	J/molxK	866.84	Joback Method
cpg	589.64	J/molxK	903.80	Joback Method
cpg	597.74	J/molxK	940.76	Joback Method
cpg	604.93	J/molxK	977.72	Joback Method
cpg	611.23	J/molxK	1014.67	Joback Method
dvisc	0.0007418	Paxs	494.29	Joback Method

dvisc	0.0004414	Paxs	544.06	Joback Method
dvisc	0.0002865	Paxs	593.84	Joback Method
dvisc	0.0001988	Paxs	643.61	Joback Method
dvisc	0.0001454	Paxs	693.38	Joback Method
dvisc	0.0001109	Paxs	743.16	Joback Method
dvisc	0.0000875	Paxs	792.93	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=U390460&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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