

Glutaric acid, 2,2-dichloroethyl 2-methyl-4-chlorophenyl ester

Inchi:	InChI=1S/C14H15Cl3O4/c1-9-7-10(15)5-6-11(9)21-14(19)4-2-3-13(18)20-8-12(16)17/h5-
InchiKey:	DDOATBNWISWWFT-UHFFFAOYSA-N
Formula:	C14H15Cl3O4
SMILES:	Cc1cc(Cl)ccc1OC(=O)CCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	353.62

Physical Properties

Property code	Value	Unit	Source
gf	-345.92	kJ/mol	Joback Method
hf	-660.80	kJ/mol	Joback Method
hfus	39.92	kJ/mol	Joback Method
hvap	81.44	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	4.071		Crippen Method
mvol	235.960	ml/mol	McGowan Method
pc	1937.24	kPa	Joback Method
rinpol	2426.00		NIST Webbook
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tb	820.79	K	Joback Method
tc	1040.75	K	Joback Method
tf	518.08	K	Joback Method
vc	0.900	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.96	J/molxK	820.79	Joback Method
cpg	658.15	J/molxK	1004.09	Joback Method
cpg	650.83	J/molxK	967.43	Joback Method
cpg	642.56	J/molxK	930.77	Joback Method
cpg	633.33	J/molxK	894.11	Joback Method
cpg	623.13	J/molxK	857.45	Joback Method
cpg	664.54	J/molxK	1040.75	Joback Method
dvisc	0.0000767	Paxs	820.79	Joback Method

dvisc	0.0000962	Paxs	770.34	Joback Method
dvisc	0.0001247	Paxs	719.89	Joback Method
dvisc	0.0001680	Paxs	669.43	Joback Method
dvisc	0.0002376	Paxs	618.98	Joback Method
dvisc	0.0003575	Paxs	568.53	Joback Method
dvisc	0.0005822	Paxs	518.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392068&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
mccvol:	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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