

Glutaric acid, monochloride, 3-chlorophenyl ester

Inchi:	InChI=1S/C11H10Cl2O3/c12-8-3-1-4-9(7-8)16-11(15)6-2-5-10(13)14/h1,3-4,7H,2,5-6H2
InchiKey:	GAWPHQWVXUGOGJ-UHFFFAOYSA-N
Formula:	C11H10Cl2O3
SMILES:	O=C(Cl)CCCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	261.10

Physical Properties

Property code	Value	Unit	Source
gf	-242.18	kJ/mol	Joback Method
hf	-434.17	kJ/mol	Joback Method
hfus	30.68	kJ/mol	Joback Method
hvap	67.69	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.181		Crippen Method
mcvol	175.580	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
rinpola	1930.00		NIST Webbook
tb	687.76	K	Joback Method
tc	912.14	K	Joback Method
tf	434.60	K	Joback Method
vc	0.671	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.13	J/molxK	687.76	Joback Method
cpg	421.11	J/molxK	725.16	Joback Method
cpg	431.28	J/molxK	762.55	Joback Method
cpg	440.66	J/molxK	799.95	Joback Method
cpg	449.28	J/molxK	837.35	Joback Method
cpg	457.15	J/molxK	874.74	Joback Method
cpg	464.30	J/molxK	912.14	Joback Method
dvisc	0.0012642	Paxs	434.60	Joback Method
dvisc	0.0007938	Paxs	476.79	Joback Method

dvisc	0.0005376	Paxs	518.99	Joback Method
dvisc	0.0003861	Paxs	561.18	Joback Method
dvisc	0.0002904	Paxs	603.37	Joback Method
dvisc	0.0002267	Paxs	645.57	Joback Method
dvisc	0.0001825	Paxs	687.76	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358826&Units=SI

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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