

Glutaric acid, monochloride, 2,3-dimethylphenyl ester

Inchi:	InChI=1S/C13H15ClO3/c1-9-5-3-6-11(10(9)2)17-13(16)8-4-7-12(14)15/h3,5-6H,4,7-8H2,
InchiKey:	NOVYBSOSXXNQJC-UHFFFAOYSA-N
Formula:	C13H15ClO3
SMILES:	Cc1cccc(OC(=O)CCCC(=O)Cl)c1C
Mol. weight [g/mol]:	254.71

Physical Properties

Property code	Value	Unit	Source
gf	-223.04	kJ/mol	Joback Method
hf	-471.18	kJ/mol	Joback Method
hfus	31.27	kJ/mol	Joback Method
hvap	68.42	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.145		Crippen Method
mcvol	191.520	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
rinpola	1953.00		NIST Webbook
tb	701.07	K	Joback Method
tc	915.99	K	Joback Method
tf	439.74	K	Joback Method
vc	0.735	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.49	J/molxK	701.07	Joback Method
cpg	499.52	J/molxK	736.89	Joback Method
cpg	511.70	J/molxK	772.71	Joback Method
cpg	523.04	J/molxK	808.53	Joback Method
cpg	533.57	J/molxK	844.35	Joback Method
cpg	543.30	J/molxK	880.17	Joback Method
cpg	552.24	J/molxK	915.99	Joback Method
dvisc	0.0010622	Paxs	439.74	Joback Method
dvisc	0.0006696	Paxs	483.30	Joback Method

dvisc	0.0004556	Paxs	526.85	Joback Method
dvisc	0.0003288	Paxs	570.40	Joback Method
dvisc	0.0002485	Paxs	613.96	Joback Method
dvisc	0.0001949	Paxs	657.52	Joback Method
dvisc	0.0001576	Paxs	701.07	Joback Method

Sources

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=U359314&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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