Glutaric acid, monochloride, 2-methoxyphenyl ester

Inchi: InChI=1S/C12H13ClO4/c1-16-9-5-2-3-6-10(9)17-12(15)8-4-7-11(13)14/h2-3,5-6H,4,7-8H

InchiKey: NWXUPWYZJYXFIQ-UHFFFAOYSA-N

Formula: C12H13ClO4

SMILES: COc1ccccc1OC(=O)CCCC(=O)Cl

Mol. weight [g/mol]: 256.68

Physical Properties

Property code	Value	Unit	Source
gf	-326.83	kJ/mol	Joback Method
hf	-571.29	kJ/mol	Joback Method
hfus	30.26	kJ/mol	Joback Method
hvap	67.94	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.536		Crippen Method
mcvol	183.300	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
rinpol	1922.00		NIST Webbook
tb	695.63	K	Joback Method
tc	910.73	K	Joback Method
tf	438.18	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.40	J/mol×K	695.63	Joback Method
cpg	473.77	J/mol×K	731.48	Joback Method
cpg	485.31	J/mol×K	767.33	Joback Method
cpg	496.02	J/mol×K	803.18	Joback Method
cpg	505.89	J/mol×K	839.03	Joback Method
cpg	514.95	J/mol×K	874.88	Joback Method
cpg	523.19	J/mol×K	910.73	Joback Method
dvisc	0.0009861	Pa×s	438.18	Joback Method
dvisc	0.0006136	Pa×s	481.09	Joback Method

dvisc	0.0004127	Pa×s	524.00	Joback Method
dvisc	0.0002947	Pa×s	566.90	Joback Method
dvisc	0.0002207	Pa×s	609.81	Joback Method
dvisc	0.0001717	Pa×s	652.72	Joback Method
dvisc	0.0001377	Pa×s	695.63	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358675&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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