Glutaric acid, 3-chlorophenyl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C18H16Cl2O5/c1-23-16-11-13(20)8-9-15(16)25-18(22)7-3-6-17(21)24-14-5-2-4

InchiKey: ASXTZBVGQVMEFQ-UHFFFAOYSA-N

Formula: C18H16Cl2O5

SMILES: COc1cc(Cl)ccc1OC(=O)CCCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 383.22

Physical Properties

Property code	Value	Unit	Source
gf	-300.09	kJ/mol	Joback Method
hf	-629.50	kJ/mol	Joback Method
hfus	44.45	kJ/mol	Joback Method
hvap	91.69	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.683		Crippen Method
mcvol	262.190	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	2888.00		NIST Webbook
rinpol	2888.00		NIST Webbook
tb	929.40	K	Joback Method
tc	1163.97	K	Joback Method
tf	609.41	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	734.42	J/mol×K	929.40	Joback Method
cpg	744.63	J/mol×K	968.50	Joback Method
cpg	753.49	J/mol×K	1007.59	Joback Method
cpg	760.99	J/mol×K	1046.69	Joback Method
cpg	767.14	J/mol×K	1085.78	Joback Method
cpg	771.95	J/mol×K	1124.88	Joback Method
cpg	775.43	J/mol×K	1163.97	Joback Method
dvisc	0.0002510	Pa×s	609.41	Joback Method

dvisc	0.0001662	Pa×s	662.74	Joback Method
dvisc	0.0001171	Pa×s	716.07	Joback Method
dvisc	0.0000866	Pa×s	769.41	Joback Method
dvisc	0.0000666	Pa×s	822.74	Joback Method
dvisc	0.0000528	Pa×s	876.07	Joback Method
dvisc	0.0000431	Pa×s	929.40	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=U393913&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