Glutaric acid, 3-chlorophenyl 5-methyl-2-methoxybenzyl ester

Inchi: InChI=1S/C19H19ClO5/c1-13-9-10-16(23-2)17(11-13)25-19(22)8-4-7-18(21)24-15-6-3-5-

InchiKey: GGOJLNLPTHXSHL-UHFFFAOYSA-N

Formula: C19H19ClO5

SMILES: COc1ccc(C)cc1OC(=O)CCCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 362.80

Physical Properties

Property code	Value	Unit	Source
gf	-279.74	kJ/mol	Joback Method
hf	-634.40	kJ/mol	Joback Method
hfus	42.84	kJ/mol	Joback Method
hvap	89.53	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.338		Crippen Method
mcvol	264.040	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	2776.00		NIST Webbook
rinpol	2776.00		NIST Webbook
tb	914.85	K	Joback Method
tc	1144.37	K	Joback Method
tf	590.76	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.95	J/mol×K	914.85	Joback Method
cpg	815.92	J/mol×K	1106.12	Joback Method
cpg	809.65	J/mol×K	1067.86	Joback Method
cpg	802.03	J/mol×K	1029.61	Joback Method
cpg	793.04	J/mol×K	991.36	Joback Method
cpg	782.68	J/mol×K	953.10	Joback Method
cpg	820.83	J/mol×K	1144.37	Joback Method
dvisc	0.0000435	Pa×s	914.85	Joback Method

dvisc	0.0000536	Pa×s	860.83	Joback Method
dvisc	0.0000679	Pa×s	806.82	Joback Method
dvisc	0.0000889	Pa×s	752.80	Joback Method
dvisc	0.0001216	Pa×s	698.79	Joback Method
dvisc	0.0001751	Pa×s	644.77	Joback Method
dvisc	0.0002695	Pa×s	590.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393930&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