Glutaric acid, hept-2-yl 2-methyl-4-chlorophenyl ester

Inchi: InChI=1S/C19H27ClO4/c1-4-5-6-8-15(3)23-18(21)9-7-10-19(22)24-17-12-11-16(20)13-14

InchiKey: QMNGXVCKRLISIK-UHFFFAOYSA-N

Formula: C19H27ClO4

SMILES: CCCCCC(C)OC(=O)CCCC(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 354.87

Physical Properties

Property code	Value	Unit	Source
gf	-279.96	kJ/mol	Joback Method
hf	-732.52	kJ/mol	Joback Method
hfus	44.48	kJ/mol	Joback Method
hvap	83.80	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	5.236		Crippen Method
mcvol	281.930	ml/mol	McGowan Method
pc	1394.37	kPa	Joback Method
rinpol	2437.00		NIST Webbook
rinpol	2437.00		NIST Webbook
tb	860.33	K	Joback Method
tc	1067.39	K	Joback Method
tf	514.59	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	845.93	J/mol×K	860.33	Joback Method
cpg	860.72	J/mol×K	894.84	Joback Method
cpg	874.36	J/mol×K	929.35	Joback Method
cpg	886.88	J/mol×K	963.86	Joback Method
cpg	898.29	J/mol×K	998.37	Joback Method
cpg	908.61	J/mol×K	1032.88	Joback Method
cpg	917.86	J/mol×K	1067.39	Joback Method
dvisc	0.0005178	Pa×s	514.59	Joback Method

dvisc	0.0002892	Pa×s	572.21	Joback Method
dvisc	0.0001797	Pa×s	629.84	Joback Method
dvisc	0.0001209	Pa×s	687.46	Joback Method
dvisc	0.0000865	Pa×s	745.08	Joback Method
dvisc	0.0000650	Pa×s	802.71	Joback Method
dvisc	0.0000507	Pa×s	860.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392070&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