Glutaric acid, 2-formyl-4-chlorophenyl pentyl ester

Other names: Glutaric acid, 2-acetyl-4-chlorophenyl pentyl ester
Inchi: InChI=1S/C17H21ClO5/c1-2-3-4-10-22-16(20)6-5-7-17(21)23-15-9-8-14(18)11-13(15)12-
InchiKey: AUFZIOAZBQNPIB-UHFFFAOYSA-N
Formula: C17H21ClO5
SMILES: CCCCCOC(=O)CCCC(=O)Oc1ccc(Cl)cc1C=O
Mol. weight [g/mol]: 340.80

Physical Properties

Property code	Value	Unit	Source
gf	-393.88	kJ/mol	Joback Method
hf	-771.54	kJ/mol	Joback Method
hfus	45.11	kJ/mol	Joback Method
hvap	86.45	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.962		Crippen Method
mcvol	255.320	ml/mol	McGowan Method
pc	1707.53	kPa	Joback Method
rinpol	2545.00		NIST Webbook
rinpol	2545.00		NIST Webbook
tb	863.67	K	Joback Method
tc	1073.45	K	Joback Method
tf	549.05	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.47	J/mol×K	863.67	Joback Method
cpg	795.01	J/mol×K	1038.49	Joback Method
cpg	786.75	J/mol×K	1003.52	Joback Method
cpg	777.47	J/mol×K	968.56	Joback Method
cpg	767.18	J/mol×K	933.60	Joback Method
cpg	755.84	J/mol×K	898.63	Joback Method
cpg	802.27	J/mol×K	1073.45	Joback Method

dvisc	0.0000791	Pa×s	863.67	Joback Method
dvisc	0.0000986	Pa×s	811.23	Joback Method
dvisc	0.0001267	Pa×s	758.80	Joback Method
dvisc	0.0001690	Pa×s	706.36	Joback Method
dvisc	0.0002360	Pa×s	653.92	Joback Method
dvisc	0.0003493	Pa×s	601.49	Joback Method
dvisc	0.0005574	Pa×s	549.05	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=U358934&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