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

Other names: Glutaric acid, 2-acetyl-4-chlorophenyl isobutyl ester
Inchi: InChI=1S/C16H19ClO5/c1-11(2)10-21-15(19)4-3-5-16(20)22-14-7-6-13(17)8-12(14)9-18/
InchiKey: DRKFRKYSWLAMIM-UHFFFAOYSA-N
Formula: C16H19ClO5
SMILES: CC(C)COC(=O)CCCC(=O)Oc1ccc(Cl)cc1C=O
Mol. weight [g/mol]: 326.77

Physical Properties

Property code	Value	Unit	Source
gf	-404.74	kJ/mol	Joback Method
hf	-756.18	kJ/mol	Joback Method
hfus	39.00	kJ/mol	Joback Method
hvap	83.84	kJ/mol	Joback Method
log10ws	-4.26		Crippen Method
logp	3.427		Crippen Method
mcvol	241.230	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	2392.00		NIST Webbook
rinpol	2392.00		NIST Webbook
tb	840.35	K	Joback Method
tc	1052.95	K	Joback Method
tf	522.78	K	Joback Method
vc	0.931	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.79	J/mol×K	840.35	Joback Method
cpg	700.03	J/mol×K	875.78	Joback Method
cpg	711.23	J/mol×K	911.22	Joback Method
cpg	721.40	J/mol×K	946.65	Joback Method
cpg	730.56	J/mol×K	982.08	Joback Method
cpg	738.71	J/mol×K	1017.52	Joback Method
cpg	745.85	J/mol×K	1052.95	Joback Method

dvisc	0.0006703	Pa×s	522.78	Joback Method
dvisc	0.0004035	Pa×s	575.71	Joback Method
dvisc	0.0002646	Pa×s	628.64	Joback Method
dvisc	0.0001852	Pa×s	681.56	Joback Method
dvisc	0.0001365	Pa×s	734.49	Joback Method
dvisc	0.0001048	Pa×s	787.42	Joback Method
dvisc	0.0000832	Pa×s	840.35	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U358932&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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