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

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

Physical Properties

Property code	Value	Unit	Source
gf	-402.30	kJ/mol	Joback Method
hf	-750.90	kJ/mol	Joback Method
hfus	42.52	kJ/mol	Joback Method
hvap	84.23	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	3.571		Crippen Method
mcvol	241.230	ml/mol	McGowan Method
pc	1851.52	kPa	Joback Method
rinpol	2441.00		NIST Webbook
tb	840.79	K	Joback Method
tc	1050.94	K	Joback Method
tf	537.78	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	687.21	J/mol×K	840.79	Joback Method
cpg	737.85	J/mol×K	1015.92	Joback Method
cpg	729.69	J/mol×K	980.89	Joback Method
cpg	720.56	J/mol×K	945.87	Joback Method
cpg	710.44	J/mol×K	910.84	Joback Method
cpg	699.32	J/mol×K	875.82	Joback Method
cpg	745.05	J/mol×K	1050.94	Joback Method
dvisc	0.0000908	Pa×s	840.79	Joback Method

dvisc	0.0001127	Pa×s	790.29	Joback Method
dvisc	0.0001442	Pa×s	739.79	Joback Method
dvisc	0.0001912	Pa×s	689.28	Joback Method
dvisc	0.0002650	Pa×s	638.78	Joback Method
dvisc	0.0003887	Pa×s	588.28	Joback Method
dvisc	0.0006124	Pa×s	537.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358933&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