Glutaric acid, 3-chlorophenyl 2-methylbutyl ester

Inchi: InChI=1S/C16H21ClO4/c1-3-12(2)11-20-15(18)8-5-9-16(19)21-14-7-4-6-13(17)10-14/h4,

InchiKey: UWSXRAFRDMAKJE-UHFFFAOYSA-N

Formula: C16H21ClO4

SMILES: CCC(C)COC(=O)CCCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 312.79

Physical Properties

Property code	Value	Unit	Source
gf	-295.59	kJ/mol	Joback Method
hf	-659.13	kJ/mol	Joback Method
hfus	37.10	kJ/mol	Joback Method
hvap	76.46	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.005		Crippen Method
mcvol	239.660	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	2197.00		NIST Webbook
rinpol	2197.00		NIST Webbook
tb	786.71	K	Joback Method
tc	995.09	K	Joback Method
tf	468.26	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.77	J/mol×K	786.71	Joback Method
cpg	689.96	J/mol×K	821.44	Joback Method
cpg	703.13	J/mol×K	856.17	Joback Method
cpg	715.28	J/mol×K	890.90	Joback Method
cpg	726.45	J/mol×K	925.63	Joback Method
cpg	736.62	J/mol×K	960.36	Joback Method
cpg	745.84	J/mol×K	995.09	Joback Method
dvisc	0.0008164	Pa×s	468.26	Joback Method

dvisc	0.0004495	Pa×s	521.34	Joback Method
dvisc	0.0002763	Pa×s	574.41	Joback Method
dvisc	0.0001845	Pa×s	627.48	Joback Method
dvisc	0.0001311	Pa×s	680.56	Joback Method
dvisc	0.0000980	Pa×s	733.63	Joback Method
dvisc	0.0000761	Pa×s	786.71	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=U391693&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