Glutaric acid, 3-chlorophenyl but-3-en-1-yl ester

Inchi: InChI=1S/C15H17ClO4/c1-2-3-10-19-14(17)8-5-9-15(18)20-13-7-4-6-12(16)11-13/h2,4,6

InchiKey: DUIASDXNKNAHKY-UHFFFAOYSA-N

Formula: C15H17ClO4

SMILES: C=CCCOC(=O)CCCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 296.75

Physical Properties

Property code	Value	Unit	Source
gf	-213.73	kJ/mol	Joback Method
hf	-507.78	kJ/mol	Joback Method
hfus	36.75	kJ/mol	Joback Method
hvap	73.95	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.535		Crippen Method
mcvol	221.270	ml/mol	McGowan Method
pc	1984.12	kPa	Joback Method
rinpol	2151.00		NIST Webbook
tb	760.95	K	Joback Method
tc	971.13	K	Joback Method
tf	470.23	K	Joback Method
vc	0.846	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.87	J/mol×K	760.95	Joback Method
cpg	651.33	J/mol×K	936.10	Joback Method
cpg	641.84	J/mol×K	901.07	Joback Method
cpg	631.47	J/mol×K	866.04	Joback Method
cpg	620.19	J/mol×K	831.01	Joback Method
cpg	608.00	J/mol×K	795.98	Joback Method
cpg	659.96	J/mol×K	971.13	Joback Method
dvisc	0.0001003	Pa×s	760.95	Joback Method
dvisc	0.0001260	Pa×s	712.50	Joback Method

dvisc	0.0001635	Pa×s	664.04	Joback Method
dvisc	0.0002212	Pa×s	615.59	Joback Method
dvisc	0.0003150	Pa×s	567.14	Joback Method
dvisc	0.0004793	Pa×s	518.68	Joback Method
dvisc	0.0007951	Pa×s	470.23	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=U394041&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