Glutaric acid, 3-methylbut-2-en-1-yl 3-chlorophenyl ester

Inchi: InChI=1S/C16H19ClO4/c1-12(2)9-10-20-15(18)7-4-8-16(19)21-14-6-3-5-13(17)11-14/h3,

InchiKey: BQZFTEJHXQCXQV-UHFFFAOYSA-N

Formula: C16H19ClO4

SMILES: CC(C)=CCOC(=O)CCCC(=O)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 310.77

Physical Properties

Property code	Value	Unit	Source
gf	-221.48	kJ/mol	Joback Method
hf	-546.42	kJ/mol	Joback Method
hfus	39.51	kJ/mol	Joback Method
hvap	76.88	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.925		Crippen Method
mcvol	235.360	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpol	2243.00		NIST Webbook
rinpol	2243.00		NIST Webbook
tb	791.19	K	Joback Method
tc	1005.30	K	Joback Method
tf	464.22	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.26	J/mol×K	791.19	Joback Method
cpg	662.89	J/mol×K	826.88	Joback Method
cpg	675.54	J/mol×K	862.56	Joback Method
cpg	687.25	J/mol×K	898.25	Joback Method
cpg	698.03	J/mol×K	933.93	Joback Method
cpg	707.93	J/mol×K	969.62	Joback Method
cpg	716.96	J/mol×K	1005.30	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390459&Units=SI

Legend

cpg:	Ideal gas heat capacity
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