Glutaric acid, 3-methylbut-2-en 2-chloro-5-methylphenyl ester

Inchi: InChI=1S/C17H21ClO4/c1-12(2)9-10-21-16(19)5-4-6-17(20)22-15-11-13(3)7-8-14(15)18/

InchiKey: NYOMVEBSQMBCSL-UHFFFAOYSA-N

Formula: C17H21ClO4

SMILES: CC(C)=CCOC(=O)CCCC(=O)Oc1cc(C)ccc1Cl

Mol. weight [g/mol]: 324.80

Physical Properties

Property code	Value	Unit	Source
gf	-222.69	kJ/mol	Joback Method
hf	-578.53	kJ/mol	Joback Method
hfus	41.71	kJ/mol	Joback Method
hvap	79.77	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.234		Crippen Method
mcvol	249.450	ml/mol	McGowan Method
pc	1683.79	kPa	Joback Method
rinpol	2341.00		NIST Webbook
rinpol	2341.00		NIST Webbook
tb	819.05	K	Joback Method
tc	1032.09	K	Joback Method
tf	488.01	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.81	J/mol×K	819.05	Joback Method
cpg	717.65	J/mol×K	854.56	Joback Method
cpg	730.50	J/mol×K	890.06	Joback Method
cpg	742.37	J/mol×K	925.57	Joback Method
cpg	753.30	J/mol×K	961.08	Joback Method
cpg	763.31	J/mol×K	996.59	Joback Method
cpg	772.43	J/mol×K	1032.09	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393419&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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