Glutaric acid, 3-methylbut-2-en-1-yl 4-chloro-2-methoxyphenyl ester

Inchi: InChI=1S/C17H21ClO5/c1-12(2)9-10-22-16(19)5-4-6-17(20)23-14-8-7-13(18)11-15(14)21

InchiKey: YPTNSHFLTZCZGV-UHFFFAOYSA-N

Formula: C17H21ClO5

SMILES: COc1cc(Cl)ccc1OC(=O)CCCC(=O)OCC=C(C)C

Mol. weight [g/mol]: 340.80

Physical Properties

Property code	Value	Unit	Source
gf	-327.69	kJ/mol	Joback Method
hf	-710.75	kJ/mol	Joback Method
hfus	42.90	kJ/mol	Joback Method
hvap	82.18	kJ/mol	Joback Method
log10ws	-4.66		Crippen Method
logp	3.934		Crippen Method
mcvol	255.320	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	2448.00		NIST Webbook
rinpol	2448.00		NIST Webbook
tb	841.47	K	Joback Method
tc	1053.92	K	Joback Method
tf	510.24	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	730.93	J/mol×K	841.47	Joback Method
cpg	744.32	J/mol×K	876.88	Joback Method
cpg	756.66	J/mol×K	912.29	Joback Method
cpg	767.94	J/mol×K	947.70	Joback Method
cpg	778.19	J/mol×K	983.10	Joback Method
cpg	787.42	J/mol×K	1018.51	Joback Method
cpg	795.63	J/mol×K	1053.92	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=U393905&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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