Glutaric acid, (2-chlorocyclohexyl)methyl 3-methylbut-2-en-1-yl ester

Inchi: InChI=1S/C17H27ClO4/c1-13(2)10-11-21-16(19)8-5-9-17(20)22-12-14-6-3-4-7-15(14)18/

InchiKey: UYHGTFWESCNMHI-UHFFFAOYSA-N

Formula: C17H27ClO4

SMILES: CC(C)=CCOC(=O)CCCC(=O)OCC1CCCCC1Cl

Mol. weight [g/mol]: 330.85

Physical Properties

Property code	Value	Unit	Source
gf	-299.10	kJ/mol	Joback Method
hf	-758.14	kJ/mol	Joback Method
hfus	41.35	kJ/mol	Joback Method
hvap	76.29	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	4.007		Crippen Method
mcvol	262.350	ml/mol	McGowan Method
pc	1518.75	kPa	Joback Method
rinpol	2371.00		NIST Webbook
rinpol	2371.00		NIST Webbook
tb	797.29	K	Joback Method
tc	1004.02	K	Joback Method
tf	439.69	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	795.67	J/mol×K	797.29	Joback Method
cpg	813.01	J/mol×K	831.75	Joback Method
cpg	829.13	J/mol×K	866.20	Joback Method
cpg	844.05	J/mol×K	900.66	Joback Method
cpg	857.79	J/mol×K	935.11	Joback Method
cpg	870.38	J/mol×K	969.57	Joback Method
cpg	881.85	J/mol×K	1004.02	Joback Method

Sources

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=U405443&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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