Glutaric acid, monochloride, 3-methylbut-3-enyl ester

Inchi: InChI=1S/C10H15ClO3/c1-8(2)6-7-14-10(13)5-3-4-9(11)12/h1,3-7H2,2H3

InchiKey: PLXBVXVPKNVJIS-UHFFFAOYSA-N

Formula: C10H15ClO3

SMILES: C=C(C)CCOC(=O)CCCC(=O)Cl

Mol. weight [g/mol]: 218.68

Physical Properties

Property code	Value	Unit	Source
gf	-262.16	kJ/mol	Joback Method
hf	-507.21	kJ/mol	Joback Method
hfus	27.65	kJ/mol	Joback Method
hvap	57.55	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.431		Crippen Method
mcvol	168.710	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	1494.00		NIST Webbook
tb	592.35	K	Joback Method
tc	784.05	K	Joback Method
tf	338.75	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.40	J/mol×K	592.35	Joback Method
cpg	409.65	J/mol×K	624.30	Joback Method
cpg	421.30	J/mol×K	656.25	Joback Method
cpg	432.34	J/mol×K	688.20	Joback Method
cpg	442.80	J/mol×K	720.15	Joback Method
cpg	452.69	J/mol×K	752.10	Joback Method
cpg	462.01	J/mol×K	784.05	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=U359960&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