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

Inchi: InChI=1S/C12H18Cl2O4/c1-9(2)6-7-17-11(15)4-3-5-12(16)18-8-10(13)14/h6,10H,3-5,7-8

InchiKey: FWPWPOKNRKZFII-UHFFFAOYSA-N

Formula: C12H18Cl2O4

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

Mol. weight [g/mol]: 297.18

Physical Properties

Property code	Value	Unit	Source
gf	-372.31	kJ/mol	Joback Method
hf	-709.94	kJ/mol	Joback Method
hfus	36.17	kJ/mol	Joback Method
hvap	69.04	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.013		Crippen Method
mcvol	215.000	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	1871.00		NIST Webbook
rinpol	1871.00		NIST Webbook
tb	705.00	K	Joback Method
tc	902.24	K	Joback Method
tf	395.12	K	Joback Method
vc	0.829	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	549.90	J/mol×K	705.00	Joback Method
cpg	562.72	J/mol×K	737.87	Joback Method
cpg	574.81	J/mol×K	770.75	Joback Method
cpg	586.16	J/mol×K	803.62	Joback Method
cpg	596.81	J/mol×K	836.49	Joback Method
cpg	606.75	J/mol×K	869.37	Joback Method
cpg	616.02	J/mol×K	902.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393538&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