Glutaric acid, hexa-1,5-dien-3-yl 2,2-dichloroethyl ester

Inchi: InChI=1S/C13H18Cl2O4/c1-3-6-10(4-2)19-13(17)8-5-7-12(16)18-9-11(14)15/h3-4,10-11H

InchiKey: CMHBCXVWJBSSJM-UHFFFAOYSA-N

Formula: C13H18Cl2O4

SMILES: C=CCC(C=C)OC(=O)CCCC(=O)OCC(Cl)Cl

Mol. weight [g/mol]: 309.19

Physical Properties

Property code	Value	Unit	Source
gf	-262.32	kJ/mol	Joback Method
hf	-592.43	kJ/mol	Joback Method
hfus	33.79	kJ/mol	Joback Method
hvap	69.50	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.177		Crippen Method
mcvol	224.790	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	1858.00		NIST Webbook
rinpol	1858.00		NIST Webbook
tb	716.76	K	Joback Method
tc	912.19	K	Joback Method
tf	406.91	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	579.24	J/mol×K	716.76	Joback Method
cpg	592.04	J/mol×K	749.33	Joback Method
cpg	604.06	J/mol×K	781.90	Joback Method
cpg	615.32	J/mol×K	814.47	Joback Method
cpg	625.83	J/mol×K	847.04	Joback Method
cpg	635.61	J/mol×K	879.62	Joback Method
cpg	644.68	J/mol×K	912.19	Joback Method
dvisc	0.0015615	Pa×s	406.91	Joback Method

dvisc	0.0007691	Pa×s	458.55	Joback Method
dvisc	0.0004372	Pa×s	510.19	Joback Method
dvisc	0.0002757	Pa×s	561.84	Joback Method
dvisc	0.0001879	Pa×s	613.48	Joback Method
dvisc	0.0001359	Pa×s	665.12	Joback Method
dvisc	0.0001030	Pa×s	716.76	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=U405277&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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