

Glutaric acid, hex-4-en-1-yl 2,2-dichloroethyl ester

Inchi:	InChI=1S/C13H20Cl2O4/c1-2-3-4-5-9-18-12(16)7-6-8-13(17)19-10-11(14)15/h2-3,11H,4
InchiKey:	WHUQHUVOTKESX-NSCUHMNNSA-N
Formula:	C13H20Cl2O4
SMILES:	CC=CCCCOC(=O)CCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	311.20

Physical Properties

Property code	Value	Unit	Source
gf	-355.34	kJ/mol	Joback Method
hf	-720.79	kJ/mol	Joback Method
hfus	40.07	kJ/mol	Joback Method
hvap	71.18	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.403		Crippen Method
mcvol	229.090	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	1989.00		NIST Webbook
rinpol	1989.00		NIST Webbook
tb	728.00	K	Joback Method
tc	921.36	K	Joback Method
tf	420.35	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	603.24	J/molxK	728.00	Joback Method
cpg	616.41	J/molxK	760.23	Joback Method
cpg	628.82	J/molxK	792.45	Joback Method
cpg	640.48	J/molxK	824.68	Joback Method
cpg	651.42	J/molxK	856.90	Joback Method
cpg	661.63	J/molxK	889.13	Joback Method
cpg	671.15	J/molxK	921.36	Joback Method
dvisc	0.0012076	Paxs	420.35	Joback Method

dvisc	0.0006120	Paxs	471.62	Joback Method
dvisc	0.0003544	Paxs	522.90	Joback Method
dvisc	0.0002262	Paxs	574.17	Joback Method
dvisc	0.0001555	Paxs	625.45	Joback Method
dvisc	0.0001131	Paxs	676.73	Joback Method
dvisc	0.0000860	Paxs	728.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405300&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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

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