

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

Inchi:	InChI=1S/C11H16Cl2O4/c1-2-3-7-16-10(14)5-4-6-11(15)17-8-9(12)13/h2,9H,1,3-8H2
InchiKey:	JUJMHWHBMMRXNP-UHFFFAOYSA-N
Formula:	C11H16Cl2O4
SMILES:	C=CCCOC(=O)CCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	283.15

Physical Properties

Property code	Value	Unit	Source
gf	-364.56	kJ/mol	Joback Method
hf	-671.30	kJ/mol	Joback Method
hfus	33.41	kJ/mol	Joback Method
hvap	66.10	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.623		Crippen Method
mvol	200.910	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	1794.00		NIST Webbook
rinpol	1794.00		NIST Webbook
tb	674.76	K	Joback Method
tc	867.70	K	Joback Method
tf	401.13	K	Joback Method
vc	0.772	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.29	J/molxK	674.76	Joback Method
cpg	510.40	J/molxK	706.92	Joback Method
cpg	521.83	J/molxK	739.07	Joback Method
cpg	532.60	J/molxK	771.23	Joback Method
cpg	542.71	J/molxK	803.39	Joback Method
cpg	552.16	J/molxK	835.54	Joback Method
cpg	560.96	J/molxK	867.70	Joback Method
dvisc	0.0015558	Paxs	401.13	Joback Method

dvisc	0.0008451	Paxs	446.74	Joback Method
dvisc	0.0005140	Paxs	492.34	Joback Method
dvisc	0.0003401	Paxs	537.94	Joback Method
dvisc	0.0002401	Paxs	583.55	Joback Method
dvisc	0.0001782	Paxs	629.15	Joback Method
dvisc	0.0001377	Paxs	674.76	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U394034&Units=SI

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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