

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

Inchi:	InChI=1S/C11H16Cl2O4/c1-3-8(2)17-11(15)6-4-5-10(14)16-7-9(12)13/h3,8-9H,1,4-7H2,2
InchiKey:	GLETVGMXLXJBAE-UHFFFAOYSA-N
Formula:	C11H16Cl2O4
SMILES:	C=CC(C)OC(=O)CCCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]:	283.15

Physical Properties

Property code	Value	Unit	Source
gf	-367.00	kJ/mol	Joback Method
hf	-676.58	kJ/mol	Joback Method
hfus	29.89	kJ/mol	Joback Method
hvap	65.72	kJ/mol	Joback Method
log10ws	-3.03		Crippen Method
logp	2.621		Crippen Method
mvol	200.910	ml/mol	McGowan Method
pc	2069.88	kPa	Joback Method
rinpol	1698.00		NIST Webbook
rinpol	1698.00		NIST Webbook
tb	674.32	K	Joback Method
tc	870.43	K	Joback Method
tf	386.13	K	Joback Method
vc	0.766	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.82	J/molxK	674.32	Joback Method
cpg	511.16	J/molxK	707.00	Joback Method
cpg	522.79	J/molxK	739.69	Joback Method
cpg	533.72	J/molxK	772.37	Joback Method
cpg	543.97	J/molxK	805.06	Joback Method
cpg	553.52	J/molxK	837.74	Joback Method
cpg	562.39	J/molxK	870.43	Joback Method
dvisc	0.0018930	Paxs	386.13	Joback Method

dvisc	0.0009420	Paxs	434.16	Joback Method
dvisc	0.0005387	Paxs	482.19	Joback Method
dvisc	0.0003409	Paxs	530.22	Joback Method
dvisc	0.0002327	Paxs	578.26	Joback Method
dvisc	0.0001685	Paxs	626.29	Joback Method
dvisc	0.0001277	Paxs	674.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405235&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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