

Glutaric acid, di(2,2,2-trichloroethyl) ester

Inchi:	InChI=1S/C9H10Cl6O4/c10-8(11,12)4-18-6(16)2-1-3-7(17)19-5-9(13,14)15/h1-5H2
InchiKey:	RJGJHHTZWFWD-BOD-UHFFFAOYSA-N
Formula:	C9H10Cl6O4
SMILES:	O=C(CCCC(=O)OCC(Cl)(Cl)Cl)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	394.89

Physical Properties

Property code	Value	Unit	Source
gf	-508.84	kJ/mol	Joback Method
hf	-830.63	kJ/mol	Joback Method
hfus	34.99	kJ/mol	Joback Method
hvap	77.66	kJ/mol	Joback Method
log10ws	-4.44		Crippen Method
logp	3.984		Crippen Method
mvol	225.990	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	2157.00		NIST Webbook
rinpol	2157.00		NIST Webbook
tb	776.02	K	Joback Method
tc	1000.02	K	Joback Method
tf	519.87	K	Joback Method
vc	0.860	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.29	J/molxK	776.02	Joback Method
cpg	546.44	J/molxK	962.69	Joback Method
cpg	541.09	J/molxK	925.36	Joback Method
cpg	535.16	J/molxK	888.02	Joback Method
cpg	528.58	J/molxK	850.69	Joback Method
cpg	521.31	J/molxK	813.35	Joback Method
cpg	551.25	J/molxK	1000.02	Joback Method
dvisc	0.0000695	Paxs	776.02	Joback Method

dvisc	0.0000897	Paxs	733.33	Joback Method
dvisc	0.0001195	Paxs	690.64	Joback Method
dvisc	0.0001653	Paxs	647.94	Joback Method
dvisc	0.0002394	Paxs	605.25	Joback Method
dvisc	0.0003669	Paxs	562.56	Joback Method
dvisc	0.0006030	Paxs	519.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359355&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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