

Glutaric acid, ethyl 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C9H13Cl3O4/c1-2-15-7(13)4-3-5-8(14)16-6-9(10,11)12/h2-6H2,1H3
InchiKey:	HEIUDQJBMQGCNV-UHFFFAOYSA-N
Formula:	C9H13Cl3O4
SMILES:	CCOC(=O)CCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	291.56

Physical Properties

Property code	Value	Unit	Source
gf	-475.89	kJ/mol	Joback Method
hf	-774.66	kJ/mol	Joback Method
hfus	29.82	kJ/mol	Joback Method
hvap	65.80	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.633		Crippen Method
mcvol	189.270	ml/mol	McGowan Method
pc	2306.95	kPa	Joback Method
rinqol	1703.00		NIST Webbook
tb	666.96	K	Joback Method
tc	871.06	K	Joback Method
tf	427.69	K	Joback Method
vc	0.724	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	447.73	J/molxK	666.96	Joback Method
cpg	458.47	J/molxK	700.98	Joback Method
cpg	468.53	J/molxK	734.99	Joback Method
cpg	477.90	J/molxK	769.01	Joback Method
cpg	486.62	J/molxK	803.03	Joback Method
cpg	494.70	J/molxK	837.05	Joback Method
cpg	502.14	J/molxK	871.06	Joback Method
dvisc	0.0012886	Paxs	427.69	Joback Method
dvisc	0.0007598	Paxs	467.57	Joback Method

dvisc	0.0004868	Paxs	507.45	Joback Method
dvisc	0.0003328	Paxs	547.33	Joback Method
dvisc	0.0002396	Paxs	587.20	Joback Method
dvisc	0.0001798	Paxs	627.08	Joback Method
dvisc	0.0001397	Paxs	666.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359343&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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