

Glutaric acid, butyl 2,2,2-trichloroethyl ester

Inchi:	InChI=1S/C11H17Cl3O4/c1-2-3-7-17-9(15)5-4-6-10(16)18-8-11(12,13)14/h2-8H2,1H3
InchiKey:	KYTFMEALQYBXSK-UHFFFAOYSA-N
Formula:	C11H17Cl3O4
SMILES:	CCCCOC(=O)CCCC(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]:	319.61

Physical Properties

Property code	Value	Unit	Source
gf	-459.05	kJ/mol	Joback Method
hf	-815.94	kJ/mol	Joback Method
hfus	35.00	kJ/mol	Joback Method
hvap	70.25	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.413		Crippen Method
mvol	217.450	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	1903.00		NIST Webbook
tb	712.72	K	Joback Method
tc	912.17	K	Joback Method
tf	450.23	K	Joback Method
vc	0.836	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	548.97	J/molxK	712.72	Joback Method
cpg	560.87	J/molxK	745.96	Joback Method
cpg	572.01	J/molxK	779.20	Joback Method
cpg	582.41	J/molxK	812.44	Joback Method
cpg	592.09	J/molxK	845.68	Joback Method
cpg	601.07	J/molxK	878.92	Joback Method
cpg	609.36	J/molxK	912.17	Joback Method
dvisc	0.0010572	Paxs	450.23	Joback Method
dvisc	0.0006051	Paxs	493.98	Joback Method

dvisc	0.0003792	Paxs	537.73	Joback Method
dvisc	0.0002549	Paxs	581.48	Joback Method
dvisc	0.0001812	Paxs	625.22	Joback Method
dvisc	0.0001347	Paxs	668.97	Joback Method
dvisc	0.0001038	Paxs	712.72	Joback Method

Sources

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=U359346&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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