

Glutaric acid, butyl 2-chloropropyl ester

Inchi:	InChI=1S/C12H21ClO4/c1-3-4-8-16-11(14)6-5-7-12(15)17-9-10(2)13/h10H,3-9H2,1-2H3
InchiKey:	JAXBVRVWYSMYEX-UHFFFAOYSA-N
Formula:	C12H21ClO4
SMILES:	CCCCOC(=O)CCCC(=O)OCC(C)Cl
Mol. weight [g/mol]:	264.75

Physical Properties

Property code	Value	Unit	Source
gf	-432.05	kJ/mol	Joback Method
hf	-801.63	kJ/mol	Joback Method
hfus	33.08	kJ/mol	Joback Method
hvap	64.62	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.671		Crippen Method
mvol	207.060	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	1787.00		NIST Webbook
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tb	663.53	K	Joback Method
tc	848.07	K	Joback Method
tf	384.24	K	Joback Method
vc	0.798	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.79	J/molxK	663.53	Joback Method
cpg	559.86	J/molxK	694.29	Joback Method
cpg	573.23	J/molxK	725.04	Joback Method
cpg	585.92	J/molxK	755.80	Joback Method
cpg	597.91	J/molxK	786.56	Joback Method
cpg	609.21	J/molxK	817.32	Joback Method
cpg	619.82	J/molxK	848.07	Joback Method
dvisc	0.0017583	Paxs	384.24	Joback Method

dvisc	0.0008988	Paxs	430.79	Joback Method
dvisc	0.0005237	Paxs	477.34	Joback Method
dvisc	0.0003359	Paxs	523.88	Joback Method
dvisc	0.0002316	Paxs	570.43	Joback Method
dvisc	0.0001690	Paxs	616.98	Joback Method
dvisc	0.0001288	Paxs	663.53	Joback Method

Sources

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=U359494&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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