

Glutaric acid, 2-chloropropyl isobutyl ester

Inchi: InChI=1S/C12H21ClO4/c1-9(2)7-16-11(14)5-4-6-12(15)17-8-10(3)13/h9-10H,4-8H2,1-3H
InchiKey: BOTXGOKCXUWFQN-UHFFFAOYSA-N
Formula: C12H21ClO4
SMILES: CC(C)COC(=O)CCCC(=O)OCC(C)Cl
Mol. weight [g/mol]: 264.75

Physical Properties

Property code	Value	Unit	Source
gf	-434.49	kJ/mol	Joback Method
hf	-806.91	kJ/mol	Joback Method
hfus	29.56	kJ/mol	Joback Method
hvap	64.23	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	2.526		Crippen Method
mcvol	207.060	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinpol	1743.00		NIST Webbook
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tb	663.09	K	Joback Method
tc	850.51	K	Joback Method
tf	369.24	K	Joback Method
vc	0.792	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	546.28	J/molxK	663.09	Joback Method
cpg	560.60	J/molxK	694.33	Joback Method
cpg	574.19	J/molxK	725.56	Joback Method
cpg	587.07	J/molxK	756.80	Joback Method
cpg	599.22	J/molxK	788.04	Joback Method
cpg	610.65	J/molxK	819.28	Joback Method
cpg	621.37	J/molxK	850.51	Joback Method
dvisc	0.0021925	Paxs	369.24	Joback Method

dvisc	0.0010164	Paxs	418.22	Joback Method
dvisc	0.0005536	Paxs	467.19	Joback Method
dvisc	0.0003384	Paxs	516.16	Joback Method
dvisc	0.0002253	Paxs	565.14	Joback Method
dvisc	0.0001600	Paxs	614.12	Joback Method
dvisc	0.0001195	Paxs	663.09	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359493&Units=SI

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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