Glutaric acid, monochloride, heptyl ester

Inchi: InChI=1S/C12H21ClO3/c1-2-3-4-5-6-10-16-12(15)9-7-8-11(13)14/h2-10H2,1H3
InchiKey: XXHHJMNRNYJBCD-UHFFFAOYSA-N
Formula: C12H21ClO3
SMILES: CCCCCCCOC(=O)CCCC(=O)Cl
Mol. weight [g/mol]: 248.75

Physical Properties

Property code	Value	Unit	Source
gf	-324.61	kJ/mol	Joback Method
hf	-664.13	kJ/mol	Joback Method
hfus	35.42	kJ/mol	Joback Method
hvap	62.59	kJ/mol	Joback Method
log10ws	-3.64		Crippen Method
logp	3.436		Crippen Method
mcvol	201.190	ml/mol	McGowan Method
pc	1893.65	kPa	Joback Method
rinpol	1722.00		NIST Webbook
tb	641.55	K	Joback Method
tc	823.79	K	Joback Method
tf	377.01	K	Joback Method
vc	0.786	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	518.47	J/mol×K	641.55	Joback Method
cpg	581.87	J/mol×K	793.41	Joback Method
cpg	570.49	J/mol×K	763.04	Joback Method
cpg	558.47	J/mol×K	732.67	Joback Method
cpg	545.81	J/mol×K	702.30	Joback Method
cpg	532.48	J/mol×K	671.92	Joback Method
cpg	592.63	J/mol×K	823.79	Joback Method
dvisc	0.0001795	Pa×s	641.55	Joback Method
dvisc	0.0002318	Pa×s	597.46	Joback Method

dvisc	0.0003120	Pa×s	553.37	Joback Method
dvisc	0.0004419	Pa×s	509.28	Joback Method
dvisc	0.0006688	Pa×s	465.19	Joback Method
dvisc	0.0011038	Pa×s	421.10	Joback Method
dvisc	0.0020482	Pa×s	377.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358338&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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