

Glutaric acid, 3-chlorophenyl ethyl ester

Inchi:	InChI=1S/C13H15ClO4/c1-2-17-12(15)7-4-8-13(16)18-11-6-3-5-10(14)9-11/h3,5-6,9H,2,4
InchiKey:	OSXYISGLRMBLAZ-UHFFFAOYSA-N
Formula:	C13H15ClO4
SMILES:	CCOC(=O)CCCC(=O)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	270.71

Physical Properties

Property code	Value	Unit	Source
gf	-318.41	kJ/mol	Joback Method
hf	-591.93	kJ/mol	Joback Method
hfus	32.85	kJ/mol	Joback Method
hvap	70.17	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.979		Crippen Method
mvol	197.390	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	1987.00		NIST Webbook
tb	718.51	K	Joback Method
tc	930.52	K	Joback Method
tf	449.45	K	Joback Method
vc	0.752	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.07	J/molxK	718.51	Joback Method
cpg	568.79	J/molxK	895.19	Joback Method
cpg	559.38	J/molxK	859.85	Joback Method
cpg	549.10	J/molxK	824.52	Joback Method
cpg	537.96	J/molxK	789.18	Joback Method
cpg	525.96	J/molxK	753.85	Joback Method
cpg	577.36	J/molxK	930.52	Joback Method
dvisc	0.0001220	Paxs	718.51	Joback Method
dvisc	0.0001527	Paxs	673.67	Joback Method

dvisc	0.0001974	Paxs	628.82	Joback Method
dvisc	0.0002654	Paxs	583.98	Joback Method
dvisc	0.0003749	Paxs	539.14	Joback Method
dvisc	0.0005638	Paxs	494.29	Joback Method
dvisc	0.0009197	Paxs	449.45	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=U358808&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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