

Glutaric acid, monochloride, 3-ethylphenyl ester

Inchi:	InChI=1S/C13H15ClO3/c1-2-10-5-3-6-11(9-10)17-13(16)8-4-7-12(14)15/h3,5-6,9H,2,4,7-
InchiKey:	BQSKDKVGTCTFPBN-UHFFFAOYSA-N
Formula:	C13H15ClO3
SMILES:	CCc1cccc(OC(=O)CCCC(=O)Cl)c1
Mol. weight [g/mol]:	254.71

Physical Properties

Property code	Value	Unit	Source
gf	-213.41	kJ/mol	Joback Method
hf	-459.71	kJ/mol	Joback Method
hfus	31.66	kJ/mol	Joback Method
hvap	67.76	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.090		Crippen Method
mcvol	191.520	ml/mol	McGowan Method
pc	2315.84	kPa	Joback Method
rinpola	1936.00		NIST Webbook
tb	696.09	K	Joback Method
tc	910.19	K	Joback Method
tf	427.22	K	Joback Method
vc	0.735	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.63	J/molxK	696.09	Joback Method
cpg	500.80	J/molxK	731.77	Joback Method
cpg	513.08	J/molxK	767.46	Joback Method
cpg	524.52	J/molxK	803.14	Joback Method
cpg	535.12	J/molxK	838.82	Joback Method
cpg	544.91	J/molxK	874.50	Joback Method
cpg	553.92	J/molxK	910.19	Joback Method
dvisc	0.0012666	Paxs	427.22	Joback Method
dvisc	0.0007593	Paxs	472.03	Joback Method

dvisc	0.0004975	Paxs	516.84	Joback Method
dvisc	0.0003487	Paxs	561.65	Joback Method
dvisc	0.0002575	Paxs	606.47	Joback Method
dvisc	0.0001983	Paxs	651.28	Joback Method
dvisc	0.0001580	Paxs	696.09	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359175&Units=SI
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

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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