

Glutaric acid, monochloride, 2-pentyl ester

Inchi:	InChI=1S/C10H17ClO3/c1-3-5-8(2)14-10(13)7-4-6-9(11)12/h8H,3-7H2,1-2H3
InchiKey:	YPYDCFWIMANHOY-UHFFFAOYSA-N
Formula:	C10H17ClO3
SMILES:	CCCC(C)OC(=O)CCCC(=O)Cl
Mol. weight [g/mol]:	220.69

Physical Properties

Property code	Value	Unit	Source
gf	-343.89	kJ/mol	Joback Method
hf	-628.13	kJ/mol	Joback Method
hfus	26.72	kJ/mol	Joback Method
hvap	57.75	kJ/mol	Joback Method
log10ws	-2.91		Crippen Method
logp	2.654		Crippen Method
mcvol	173.010	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinpol	1436.00		NIST Webbook
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tb	595.35	K	Joback Method
tc	784.22	K	Joback Method
tf	339.47	K	Joback Method
vc	0.668	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	418.71	J/molxK	595.35	Joback Method
cpg	477.53	J/molxK	752.74	Joback Method
cpg	466.98	J/molxK	721.27	Joback Method
cpg	455.83	J/molxK	689.79	Joback Method
cpg	444.07	J/molxK	658.31	Joback Method
cpg	431.70	J/molxK	626.83	Joback Method
cpg	487.50	J/molxK	784.22	Joback Method
dvisc	0.0002108	Paxs	595.35	Joback Method

dvisc	0.0002758	Paxs	552.70	Joback Method
dvisc	0.0003776	Paxs	510.06	Joback Method
dvisc	0.0005473	Paxs	467.41	Joback Method
dvisc	0.0008548	Paxs	424.76	Joback Method
dvisc	0.0014748	Paxs	382.12	Joback Method
dvisc	0.0029181	Paxs	339.47	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=U358213&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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