

Glutaric acid, di(2-(2-chlorophenoxy)ethyl) ester

Inchi:	InChI=1S/C22H24Cl2O5/c23-18-9-2-1-7-17(18)8-6-14-28-21(25)12-5-13-22(26)29-16-15
InchiKey:	IHNVMCUWDMUCJE-UHFFFAOYSA-N
Formula:	C22H24Cl2O5
SMILES:	O=C(CCCC(=O)OCCOc1ccccc1Cl)OCCc1ccccc1Cl
Mol. weight [g/mol]:	439.33

Physical Properties

Property code	Value	Unit	Source
gf	-256.78	kJ/mol	Joback Method
hf	-700.59	kJ/mol	Joback Method
hfus	55.20	kJ/mol	Joback Method
hvap	99.93	kJ/mol	Joback Method
log10ws	-6.07		Crippen Method
logp	5.262		Crippen Method
mvol	318.550	ml/mol	McGowan Method
pc	1374.80	kPa	Joback Method
rinpol	3426.00		NIST Webbook
tb	1015.94	K	Joback Method
tc	1249.51	K	Joback Method
tf	641.97	K	Joback Method
vc	1.216	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	965.99	J/molxK	1015.94	Joback Method
cpg	976.41	J/molxK	1054.87	Joback Method
cpg	985.33	J/molxK	1093.80	Joback Method
cpg	992.79	J/molxK	1132.72	Joback Method
cpg	998.80	J/molxK	1171.65	Joback Method
cpg	1003.40	J/molxK	1210.58	Joback Method
cpg	1006.63	J/molxK	1249.51	Joback Method
dvisc	0.0001775	Paxs	641.97	Joback Method
dvisc	0.0001088	Paxs	704.30	Joback Method

dvisc	0.0000723	Paxs	766.63	Joback Method
dvisc	0.0000510	Paxs	828.95	Joback Method
dvisc	0.0000378	Paxs	891.28	Joback Method
dvisc	0.0000292	Paxs	953.61	Joback Method
dvisc	0.0000232	Paxs	1015.94	Joback Method

Sources

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=U377319&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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