

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

Inchi:	InChI=1S/C21H22Cl2O4/c22-18-8-3-1-6-16(18)12-14-26-20(24)10-5-11-21(25)27-15-13-
InchiKey:	NOVIZNMNCLQWFT-UHFFFAOYSA-N
Formula:	C21H22Cl2O4
SMILES:	O=C(CCCC(=O)OCCc1ccccc1Cl)OCCc1ccccc1Cl
Mol. weight [g/mol]:	409.30

Physical Properties

Property code	Value	Unit	Source
gf	-160.20	kJ/mol	Joback Method
hf	-547.73	kJ/mol	Joback Method
hfus	51.42	kJ/mol	Joback Method
hvap	95.30	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	5.035		Crippen Method
mcvol	298.590	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
rinqol	3154.00		NIST Webbook
tb	970.64	K	Joback Method
tc	1202.13	K	Joback Method
tf	608.47	K	Joback Method
vc	1.141	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.37	J/molxK	970.64	Joback Method
cpg	927.02	J/molxK	1163.55	Joback Method
cpg	920.50	J/molxK	1124.96	Joback Method
cpg	912.82	J/molxK	1086.38	Joback Method
cpg	903.93	J/molxK	1047.80	Joback Method
cpg	893.80	J/molxK	1009.22	Joback Method
cpg	932.44	J/molxK	1202.13	Joback Method
dvisc	0.0000366	Paxs	970.64	Joback Method
dvisc	0.0000459	Paxs	910.28	Joback Method

dvisc	0.0000595	Paxs	849.92	Joback Method
dvisc	0.0000803	Paxs	789.56	Joback Method
dvisc	0.0001139	Paxs	729.19	Joback Method
dvisc	0.0001721	Paxs	668.83	Joback Method
dvisc	0.0002820	Paxs	608.47	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=U377279&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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