

Glutaric acid, 3-chlorophenyl diphenylmethyl ester

Inchi:	InChI=1S/C24H21ClO4/c25-20-13-7-14-21(17-20)28-22(26)15-8-16-23(27)29-24(18-9-3-
InchiKey:	ZTMOEITYEWINNX-UHFFFAOYSA-N
Formula:	C24H21ClO4
SMILES:	O=C(CCCC(=O)OC(c1ccccc1)c1ccccc1)Oc1cccc(Cl)c1
Mol. weight [g/mol]:	408.87

Physical Properties

Property code	Value	Unit	Source
gf	-3.41	kJ/mol	Joback Method
hf	-351.19	kJ/mol	Joback Method
hfus	45.90	kJ/mol	Joback Method
hvap	98.82	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.748		Crippen Method
mvol	304.860	ml/mol	McGowan Method
pc	1624.60	kPa	Joback Method
rinpol	3154.00		NIST Webbook
rinpol	3154.00		NIST Webbook
tb	1023.11	K	Joback Method
tc	1274.04	K	Joback Method
tf	611.26	K	Joback Method
vc	1.147	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.28	J/molxK	1023.11	Joback Method
cpg	939.93	J/molxK	1064.93	Joback Method
cpg	949.15	J/molxK	1106.75	Joback Method
cpg	957.01	J/molxK	1148.57	Joback Method
cpg	963.61	J/molxK	1190.39	Joback Method
cpg	969.05	J/molxK	1232.21	Joback Method
cpg	973.41	J/molxK	1274.04	Joback Method
dvisc	0.0002659	Paxs	611.26	Joback Method

dvisc	0.0001476	Paxs	679.90	Joback Method
dvisc	0.0000912	Paxs	748.54	Joback Method
dvisc	0.0000612	Paxs	817.18	Joback Method
dvisc	0.0000436	Paxs	885.83	Joback Method
dvisc	0.0000327	Paxs	954.47	Joback Method
dvisc	0.0000254	Paxs	1023.11	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=U393348&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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