

Glutaric acid, 4-chloro-3-methylphenyl 4-biphenyl ester

Inchi:	InChI=1S/C24H21ClO4/c1-17-16-21(14-15-22(17)25)29-24(27)9-5-8-23(26)28-20-12-10-
InchiKey:	JQQJDIMEXZMJAT-UHFFFAOYSA-N
Formula:	C24H21ClO4
SMILES:	<chem>Cc1cc(OC(=O)CCCC(=O)Oc2ccc(-c3ccccc3)cc2)ccc1Cl</chem>
Mol. weight [g/mol]:	408.87

Physical Properties

Property code	Value	Unit	Source
gf	-20.23	kJ/mol	Joback Method
hf	-368.85	kJ/mol	Joback Method
hfus	48.64	kJ/mol	Joback Method
hvap	100.53	kJ/mol	Joback Method
log10ws	-7.93		Crippen Method
logp	5.997		Crippen Method
mcvol	304.860	ml/mol	McGowan Method
pc	1575.95	kPa	Joback Method
rinpola	3433.00		NIST Webbook
rinpola	3433.00		NIST Webbook
tb	1033.51	K	Joback Method
tc	1283.43	K	Joback Method
tf	651.30	K	Joback Method
vc	1.153	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	925.50	J/molxK	1033.51	Joback Method
cpg	935.75	J/molxK	1075.16	Joback Method
cpg	944.52	J/molxK	1116.82	Joback Method
cpg	951.88	J/molxK	1158.47	Joback Method
cpg	957.89	J/molxK	1200.12	Joback Method
cpg	962.63	J/molxK	1241.78	Joback Method
cpg	966.16	J/molxK	1283.43	Joback Method
dvisc	0.0002067	Paxs	651.30	Joback Method

dvisc	0.0001294	Paxs	715.00	Joback Method
dvisc	0.0000874	Paxs	778.70	Joback Method
dvisc	0.0000627	Paxs	842.40	Joback Method
dvisc	0.0000471	Paxs	906.11	Joback Method
dvisc	0.0000368	Paxs	969.81	Joback Method
dvisc	0.0000296	Paxs	1033.51	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=U390129&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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