

Glutaric acid, 3-chlorophenyl 4-biphenyl ester

Inchi: InChI=1S/C23H19ClO4/c24-19-8-4-9-21(16-19)28-23(26)11-5-10-22(25)27-20-14-12-18(23)
InchiKey: DYLPJCHPKNZRCF-UHFFFAOYSA-N
Formula: C23H19ClO4
SMILES: O=C(CCCC(=O)Oc1cccc(Cl)c1)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 394.85

Physical Properties

Property code	Value	Unit	Source
gf	-19.02	kJ/mol	Joback Method
hf	-336.74	kJ/mol	Joback Method
hfus	46.44	kJ/mol	Joback Method
hvap	97.64	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	5.688		Crippen Method
mvol	290.770	ml/mol	McGowan Method
pc	1724.59	kPa	Joback Method
rinpol	3311.00		NIST Webbook
rinpol	3311.00		NIST Webbook
tb	1005.65	K	Joback Method
tc	1256.24	K	Joback Method
tf	627.51	K	Joback Method
vc	1.097	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.10	J/molxK	1005.65	Joback Method
cpg	879.56	J/molxK	1047.41	Joback Method
cpg	888.59	J/molxK	1089.18	Joback Method
cpg	896.25	J/molxK	1130.94	Joback Method
cpg	902.62	J/molxK	1172.71	Joback Method
cpg	907.78	J/molxK	1214.47	Joback Method
cpg	911.80	J/molxK	1256.24	Joback Method
dvisc	0.0002527	Paxs	627.51	Joback Method

dvisc	0.0001545	Paxs	690.53	Joback Method
dvisc	0.0001026	Paxs	753.56	Joback Method
dvisc	0.0000726	Paxs	816.58	Joback Method
dvisc	0.0000539	Paxs	879.60	Joback Method
dvisc	0.0000417	Paxs	942.63	Joback Method
dvisc	0.0000333	Paxs	1005.65	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=U390128&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ 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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